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(54) Title: THREE-DIMENSIONAL STRUCTURE OF DIPEPTIDYL PEPTIDASE IV

(57) Abstract: A crystal of a dipeptidyl peptidase IV; a three-dimensional structural coordinate of the dipeptidyl peptidase IV; a method for obtaining a three-dimensional coordinate of a homolog protein of the dipeptidyl peptidase IV; a method for obtaining a three-dimensional structural coordinate of a crystal of a complex of the dipeptidyl peptidase IV and a effector of the dipeptidyl peptidase IV; a method for identifying pharmacophore of the effector of the dipeptidyl peptidase IV; a method for designing, identifying, evaluating or searching; the effector; and a program and a medium therefor for use of the three-dimensional structural coordinate.

PCT/JP2003/009523 WO 2004/011640

DESCRIPTION

THREE-DIMENSIONAL STRUCTURE OF DIPEPTIDYL PEPTIDASE IV

TECHNICAL FIELD 5

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The present invention relates to a crystal and a three-dimensional structural coordinate of a dipeptidyl peptidase IV, and an application thereof. More specifically, the present invention relates to a crystal and a threedimensional structural coordinate, a method for obtaining a three-dimensional structural coordinate of a homolog protein of a dipeptidyl peptidase IV, a method for obtaining a three-dimensional structural coordinate of a crystal of a complex of a dipeptidyl peptidase IV with an effector (e.g. inhibitor) of the dipeptidyl peptidase IV, a method for identifying a pharmacophore of an effector (e.g. inhibitor) of for the dipeptidyl peptidase IV, a method for identifying sites affecting the activity of the dipeptidyl peptidase IV, a method for designing, identifying, evaluating or searching an effector (e.g. inhibitor) of the dipeptidyl peptidase IV, and a program and a medium therefor for use of the three-dimensional structural coordinate, which are useful in the development of an effector (e.g. inhibitor) of the dipeptidyl peptidase IV, useful as a modulatory agent of immune response and as a therapeutic or prophylactic agent for diabetes, inflammation, multiple sclerosis, Graves' disease, chronic rheumatoid arthritis, AIDS, cancer and the like; and an effector (e.g. inhibitor) of the dipeptidyl peptidase IV useful as a modulatory agent of immune response and as a therapeutic or prophylactic agent for diabetes, inflammation, multiple sclerosis, Graves' disease, chronic rheumatoid arthritis, AIDS, cancer and the like.

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BACKGROUND ART

Dipeptidyl peptidase IV (hereinafter also referred to as DPPIV) is a cell membrane protein, which has been found in epithelial cell of small intestine, prostate gland, renal tubule, biliary tract and the like, activated T-cell, B-cell, NK-cell and the like. In the DPPIV, deduced active sites of DPPIV in the C-terminal side are located in extracellular portions and those in the N-terminal side are located in cytoplasm in a living body. Also, there has been suggested the relationship of the above-mentioned DPPIV with the activities of various cytokines such as interleukin-1β, interleukin-2, interleukin-3, interleukin-5, interleukin-6, interleukin-13, tumor necrosis factor-β and the like, and activities of various chemokines such as RANTES and the like in immune system [Rinsho Menneki (Clinical Immunology), 34, Revised and Enlarged Edition 19, 45-53, published by Kagaku Hyoronsha (2000), and the like].

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As to the dipeptidyl peptidase IV, it has been shown that some amino acid residues can be involved in exhibition of the activity of the dipeptidyl peptidase IV by experiments such as biochemical experiments using inhibitors, experiments using mutants produced by site-directed mutagenesis [for example, see Misumi et al, *Biochim. Biophys. Acta*, 1131, 333-336 (1992), Ogata et al, *Biochemistry*, 31, 2582-2587 (1992) and the like].

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However, it is difficult to know the three-dimensional structures for active sites from the information. Therefore, it is presently difficult to obtain the three-dimensional structural information for identifying, searching, evaluating or designing an interaction of the dipeptidyl peptidase IV and a compound that acts with the dipeptidyl peptidase IV on the level of three-dimensional structure and a

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novel compound capable of binding with and acting on the dipeptidyl peptidase IV.

DISCLOSURE OF INVENTION

A first object of the present invention is to provide a crystal of a dipeptidyl peptidase IV, which is useful for providing a three-dimensional structural coordinate as the information for designing, identifying, evaluating or searching an effector (e.g. inhibitor) of the dipeptidyl peptidase IV useful as a modulatory agent of immune response and as a therapeutic or prophylactic agent for diabetes, inflammation, multiple sclerosis, Graves' disease, chronic rheumatoid arthritis, AIDS, cancer and the like. A second object of the present invention is to provide a three-dimensional structural coordinate of the crystal. which can provide the information for designing, identifying, evaluating or searching an effector (e.g. inhibitor) of the dipeptidyl peptidase IV useful as a modulatory agent of immune response and as a therapeutic or prophylactic agent for diabetes, inflammation, multiple sclerosis, Graves' disease, chronic rheumatoid arthritis, AIDS, cancer and the like. A third object of the present invention is to provide a method for obtaining a three-dimensional structural coordinate of a homolog protein of the dipeptidyl peptidase IV, whereby refinement of a three-dimensional structural coordinate of a homolog protein of the dipeptidyl peptidase IV can be more readily performed. Furthermore, a fourth object of the present invention is to provide a method for obtaining a three-dimensional structural coordinate of a crystal of a complex of a dipeptidyl peptidase IV and an effector (e.g. inhibitor) of the dipeptidyl peptidase IV, which can provide the information for designing, identifying, evaluating or searching an

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effector (e.g. inhibitor) of the dipeptidyl peptidase IV which is useful as a modulatory agent of immune response and as a therapeutic or prophylactic agent for diabetes, inflammation, multiple sclerosis, Graves' disease, chronic rheumatoid arthritis, AIDS, cancer and the like, and is excellent in avidity. biological activity, biological stability, absorbency to a living body, and which can favorably act on the dipeptidyl peptidase IV. A fifth object of the present invention is to provide a method for identifying a pharmacophore of the dipeptidyl peptidase IV and the effector (e.g. inhibitor) of the dipeptidyl peptidase IV, which can provide the information for designing, identifying, evaluating or searching an effector (e.g. inhibitor) of the dipeptidyl peptidase IV useful as a modulatory agent of immune response and as a therapeutic or prophylactic agent for diabetes, inflammation, multiple sclerosis, Graves' disease, chronic rheumatoid arthritis, AIDS, cancer and the like, and is excellent in avidity, biological activity, biological stability, absorbency in a living body, and which can be favorably act on the dipeptidyl peptidase IV. A sixth object of the present invention is to provide a method for designing, identifying, evaluating or searching the effector (e.g. inhibitor) of the dipeptidyl peptidase IV, which can logically and conveniently provide the effector (e.g. inhibitor) of the dipeptidyl peptidase IV useful as a modulatory agent of immune response and as a therapeutic or prophylactic agent for diabetes, inflammation, multiple sclerosis, Graves' disease, chronic rheumatoid arthritis, AIDS, cancer and the like, and is excellent in avidity, biological activity, biological stability, absorbency in a living body (in vivo), and which can be favorably act on the dipeptidyl peptidase IV. A seventh object of the present invention is to provide the effector (e.g. inhibitor) of the dipeptidyl peptidase IV useful as a modulatory agent of immune

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response and as a therapeutic or prophylactic agent for diabetes, inflammation, multiple sclerosis, Graves' disease, chronic rheumatoid arthritis, AIDS, cancer and the like. An eighth object of the present invention is to provide a program and a medium therefor, which can rapidly and conveniently perform design, identification, evaluation or search of the effector (e.g. inhibitor) of the dipeptidyl peptidase IV.

Concretely, the present invention relates to:

- [1] a crystal of a dipeptidyl peptidase IV, having characteristics sufficient to ensure a resolution capable of analyzing its three-dimensional structure up to the side chain level by X-ray crystallographic structural analysis;
- [2] the crystal according to the above [1], wherein the dipeptidyl peptidase IV is a soluble polypeptide comprising a region located at extramembrane in a full-length human dipeptidyl peptidase IV;
- [3] the crystal according to the above [1] or [2], wherein the dipeptidyl peptidase IV is a polypeptide having an amino acid sequence in which a transmembrane region is deleted from the amino acid sequence of SEQ ID NO: 2, and a tag peptide is optionally added to a C-terminal side or N-terminal side thereof;
- [4] the crystal according to any one of the above [1] to [3], wherein the crystal has a space group of $P2_12_12_1$, and a lattice constant of the unit cell of $|a| = 118.0 \pm 5.0$ Å, $|b| = 125.9 \pm 5.0$ Å, $|c| = 136.8 \pm 5.0$ Å, and $\alpha = \beta = \gamma = 90^\circ$, and is orthorhombic;
 - [5] the crystal according to any one of the above [1] to [4], wherein the crystal has the structural coordinate shown in Figure 4;
- 25 [6] the crystal according to any one of the above [1] to [4], wherein the

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crystal has a structural coordinate different from the structural coordinate as shown in Figure 4 via fluctuation of a protein;

- [7] a three-dimensional structural coordinate of a dipeptidyl peptidase IV, comprising the structural coordinate shown in Figure 4;
- 5 [8] a three-dimensional structural coordinate of a dipeptidyl peptidase IV, comprising a structural coordinate different from the structural coordinate as shown in Figure 4 via fluctuation of a protein;
 - [9] the three-dimensional structural coordinate according to the above [8], wherein the fluctuation of a protein is a state that is caused by molecular oscillation or temperature, and exhibits an activity for the dipeptidyl peptidase IV in a living body;
 - [10] the three-dimensional structural coordinate according to any one of the above [7] to [9], wherein the dipeptidyl peptidase IV is a soluble polypeptide comprising a region located at extramembrane in a full-length human dipeptidyl peptidase IV;
 - [11] the three-dimensional structural coordinate according to any one of the above [7] to [10], wherein the dipeptidyl peptidase IV is a polypeptide having an amino acid sequence in which a transmembrane region is deleted from the amino acid sequence of SEQ ID NO: 2, and a tag peptide is optionally added of to a C-terminal side or N-terminal side thereof;
 - [12] a three-dimensional structural coordinate of a region in a dipeptidyl peptidase IV, comprising the three-dimensional structural coordinate of the region selected from the group consisting of the following (a) to (d):
 - (a) a region characterized by Ser 630, Asp 708 and His 740 in the amino acid sequence of SEQ ID NO: 2, and

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all or a part of a group of the amino acid residues located in the adjacent area of each of the Ser 630, Asp 708 and His 740 in the structural coordinate shown in Figure 4 or the three-dimensional structure model defined by the structural coordinate;

- 5 (b) a region characterized by Ser 630, Asp 708 and His 740 in the amino acid sequence of SEQ ID NO: 2, and all or a part of a group of the amino acid residues comprising amino acids capable of maintaining physicochemical characteristics physiologically equivalent to each of amino acids in the group of the amino acid residues located in the adjacent area of each of Ser 630, Asp 708 and His 740, in the structural coordinate shown in Figure 4 or the three-dimensional structure model defined by the structural coordinate,
 - (c) a region characterized by a group of amino acid residues comprising amino acids capable of maintaining physicochemical characteristics physiologically equivalent to each of Ser 630, Asp 708 and His 740 in the amino acid sequence of SEQ ID NO: 2, and all or a part of a group of the amino acid residues located in the adjacent area of said group of the amino acid residues in the structural coordinate shown in Figure 4 or the three-dimensional structure model defined by the structural coordinate; and
 - (d) a region characterized by a group of amino acid residues comprising amino acids capable of maintaining physicochemical characteristics physiologically equivalent to each of Ser 630, Asp 708 and His 740 in the amino acid sequence of SEQ ID NO: 2, and all or a part of a group of amino acid residues comprising amino acids

capable of maintaining physicochemical characteristics physiologically equivalent to each of the amino acids in the group of the amino acid residues located in the adjacent area of said group of the amino acids, in the structural coordinate shown in Figure 4 or the three-dimensional structure model defined by the structural coordinate,

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wherein the region in the dipeptidyl peptidase IV is a region involved in binding or interaction between the dipeptidyl peptidase IV and an effector of the dipeptidyl peptidase IV;

- [13] the three-dimensional coordinate according to the above [12], wherein the physicochemical characteristic is selected from the group consisting of features in shape of a three-dimensional structure, hydrophobicity, electric charge and pK;
- [14] a method for obtaining a three-dimensional coordinate of a homolog protein of a dipeptidyl peptidase IV, characterized in refining an electron density map of the homolog protein of the dipeptidyl peptidase IV comprising the amino acid sequence of SEQ ID NO: 2, based on all and/or a part of the three-dimensional coordinate of any one of the above [7] to [13], to give a three-dimensional structural coordinate;
- [15] a method for obtaining a three-dimensional structural coordinate of a crystal of a complex of a dipeptidyl peptidase IV and an effector of the dipeptidyl peptidase IV characterized in using all and/or a part of the three-dimensional structural coordinate of any one of the above [7] to [13], to give a three-dimensional structural coordinate;
- [16] a method for identifying pharmacophore of an effector of the dipeptidyl peptidase IV, characterized in identifying the pharmacophore based on all and/or

a part of the three-dimensional structural coordinate of any one of the above [7] to [13], and the steric conformation of the effector of the dipeptidyl peptidase IV; [17] a method for designing, identifying, evaluating or searching an effector of a dipeptidyl peptidase IV, characterized in designing, identifying, evaluating or searching a compound capable of acting on the dipeptidyl peptidase IV, based on all and/or a part of the three-dimensional structural coordinate of any one of the above [7] to [13];

- [18] the method according to the above [17], wherein the method for designing, identifying, evaluating or searching an effector comprises the steps of:
- (i) identifying a region to be targeted for binding or interaction with the effector in a dipeptidyl peptidase IV, based on all and/or a part of the three-dimensional structural coordinate according to any one of the above [7] to [13] and the steric conformation of the effector of the dipeptidyl peptidase IV;
- 15 (ii) identifying atoms or atomic groups capable of generating in the above region at least one intermolecular interaction selected from the group consisting of covalent bond, ionic interaction, ion-dipole interaction, dipole-dipole interaction, hydrogen bonding, van der Waals force, electrostatic interaction and hydrophobic interaction, with the atoms or atomic groups existing in a candidate compound; and
 - (iii) designing a compound based on the information of the above step (i) and/or (ii);
 - [19] the method according to the above [18], wherein the method further comprises the steps of:
- 25 detecting an interaction between the dipeptidyl peptidase IV and the

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designed, identified, evaluated or searched candidate compound, wherein when an interaction is detected, the candidate compound is identified as a compound capable of binding to the dipeptidyl peptidase IV, based on a degree of the interaction as an index;

[20] the method according to the above [18] or [19], wherein the method further comprises the steps of:

contacting the dipeptidyl peptidase IV with the designed, identified, evaluated or searched candidate compound and measuring the activity of the dipeptidyl peptidase IV,

- wherein when an activity increases or decreases, the designed, identified, evaluated or searched candidate compound is identified as a compound having enhancing action or inhibitory action on the activity of the dipeptidyl peptidase IV, based on a degree of the increase or decrease as an index;
 - [21] an effector of the dipeptidyl peptidase IV obtainable by the method of any one of the above [17] to [20];
 - [22] a program and a medium therefor for use of the three-dimensional structural coordinate of any one of the above [7] to [13], wherein all and/or a part of the three-dimensional structural coordinate of any one of the above [7] to [13] is recorded;
- 20 [23] the program and the medium according to the above [22], comprising a means for identifying, searching, evaluating or designing a compound capable of binding to the dipeptidyl peptidase IV or a compound having an enhancing action or inhibitory action on the activity for the dipeptidyl peptidase IV; and [24] the program and the medium according to the above [23], further comprising a means for displaying a three-dimensional graphic display of a

molecule.

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BRIEF DESCRIPTION OF THE DRAWINGS

Figure 1 is a photomicrograph of a crystal of a dipeptidyl peptidase IV, wherein the field of view is $4000 \ \mu m \times 3000 \ \mu m$.

Figure 2 is a photograph for X-ray diffraction pattern of a crystal of dipeptidyl peptidase IV.

Figure 3 is a photograph showing a three-dimensional structure of a crystal of a dipeptidyl peptidase IV displayed by the program QUANTA (Accelrys, Inc.).

Figure 4 is a drawing showing a three-dimensional coordinate of a crystal of a dipeptidyl peptidase IV.

BEST MODE FOR CARRYING OUT THE INVENTION

In the present specification, amino acid residues are expressed by using the following abbreviations, which have been adopted by the IUPAC-IUB Commission on Biochemical Nomenclature (CBN). Also, unless explicitly otherwise indicated, the amino acid sequences of peptides and proteins are identified from N-terminal to C-terminal, left terminal to right terminal, the N-terminal being identified as a first residue. Ala: alanine residue; Asp: aspartate residue; Glu: glutamate residue; Phe: phenylalanine residue; Gly: glycine residue; His: histidine residue; Ile: isoleucine residue; Lys: lysine residue; Leu: leucine residue; Met: methionine residue; Asn: asparagine residue; Pro: proline residue; Gln: glutamine residue; Arg: arginine residue; Ser: serine residue; Thr: threonine residue; Val: valine residue; Trp: tryptophane residue;

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Tyr: tyrosine residue; Cys: cysteine residue.

The crystal of the present invention is a crystal of a dipeptidyl peptidase IV, having a characteristic sufficient to ensure a resolution capable of analyzing its three-dimensional structure up to the side chain level by X-ray crystallographic structural analysis.

The "characteristic sufficient to ensure a resolution capable of analyzing three-dimensional structure up to the side chain level" is, for example,

- (1) being in a state that a molecule in a unit cell of a crystal has repeats with high regularity, namely, providing diffraction at high resolution;
- 10 (2) having suitable form and size; it is desired that for example, a crystal has at least one side grown to about 0.2 to about 0.5 mm, preferably a cubic crystal having three sides that have similarly grown, or a needle-shaped crystal having a width or thickness of about 0.2 mm or more;
 - (3) having chemical stability, dynamic stability and physical stability; and the like. In a case of the dipeptidyl peptidase IV, which is a polypeptide having a relatively large molecular weight, the term means characteristics sufficient to ensure a resolution of 3Å or less, preferably 2.8Å or less, more preferably 2.6Å or less.

The dipeptidyl peptidase IV used for the preparation of the crystal of the present invention may have a high purity sufficient for forming the crystal. In the present invention, the dipeptidyl peptidase IV used for the preparation of the crystal includes a soluble polypeptide consisting of a region located at extramembrane in a full-length human dipeptidyl peptidase IV, for example, a polypeptide in which a transmembrane region in the N-terminal side [namely the region including the transmembrane sites (the region containing at least the

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amino acid nos: 1-28 of SEQ ID NO: 2, preferably the region of the amino acid nos: 1-32)] is deleted from the amino acid sequence of a full-length human dipeptidyl peptidase IV of SEQ ID NO: 2, and a tag peptide is optionally added to a C-terminal side or N-terminal side of the amino acid sequence. Concrete examples include (I) a polypeptide in which a transmembrane region in the N-terminal side is deleted from the amino acid sequence of a full-length human dipeptidyl peptidase IV of SEQ ID NO: 2; and (II) a polypeptide in which a tag peptide is added to a C-terminal side or N-terminal side of the polypeptide of the above (I). In the polypeptide, since the transmembrane site is deleted therefrom, the polypeptide has excellent characteristics that anchoring to the membrane can be prevented, and the polypeptide is a secretory type and soluble. The tag peptide is not particularly limited. For example, a polyhistidine peptide (an oligopeptide consisting of 4 to 20 of histidine residues) or the like can be preferably used as the tag peptide.

SEQ ID NO: 2 shows the amino acid sequence of a full-length dipeptidyl peptidase IV of human colon.

The full-length dipeptidyl peptidase IV means a polypeptide of a dipeptidyl peptidase IV containing a region comprising a transmembrane site in the N-terminal side. The full-length dipeptidyl peptidase IV includes a polypeptide comprising the amino acid sequence of SEQ ID NO: 2, without being limited thereto, and encompasses its naturally occurring variant, artificially modified variant, a homolog and an ortholog derived from heterogeneous organism, and the like.

Concretely, the full-length dipeptidyl peptidase IV, besides the polypeptide comprising the amino acid sequence of SEQ ID NO: 2, includes

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conservative substitution variants, naturally occurring allelic variants and the like. Also, the full-length dipeptidyl peptidase IV includes a polypeptide having at least one, namely one or more conservative amino acid substitutions, as compared to the polypeptide comprising the amino acid sequence of SEQ ID NO: 2.

The polypeptide as described above may be a polypeptide having biological activities (namely dipeptidyl peptidase IV activity) similar to the polypeptide comprising the amino acid sequence of SEQ ID NO: 2. Concretely, there are included, for instance, a polypeptide having homology of usually about 80% or more, preferably about 90% or more, more preferably about 95% or more on the amino acid level, as compared to the full-length amino acid sequence of SEQ ID NO: 2; a polypeptide encoded by a nucleic acid capable of hybridizing with a nucleic acid consisting of the nucleotide sequence of SEQ ID NO: 1 (nucleotide sequence encoding a full-length dipeptidyl peptidase IV of human colon), under stringent conditions, or a complement thereof; and a polypeptide having deletion, substitution or addition of at least one amino acid, namely one or plural amino acids, preferably one or several amino acids in the amino acid sequence of SEQ ID NO: 2.

The number of deletion, substitution or addition of the amino acids may be to an extent that the biological activities [namely, dipeptidyl peptidase IV activity] are not lost, usually in the number of 1 to about 150, preferably 1 to about 75, more preferably 1 to about 40.

The crystallization is carried out by making a solution containing the desired protein (referred to as a protein solution) supersaturated state, based on the characteristics that the protein in solution state converts to non-soluble state

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and precipitates as a crystal when specific conditions are satisfied. Concretely, the protein can be precipitated by the following procedures 1. or 2.:

- 1. elevating the effective concentration of the protein:
- concretely, adding a precipitant such as a salt, polyethylene glycol or an organic solvent to a protein solution; reducing an amount of a solvent in the protein solution by evaporation or the like; or the like.
 - 2. reducing a repulsive force, or increasing an attractive force between protein molecules:

concretely, adding an organic solvent such as an alcohol to a protein solution; changing a hydrogen ion concentration (pH) or temperature of the protein solution; or the like.

As the conditions for the crystallization, physical and chemical factors such as a hydrogen ion concentration (pH), a kind of buffer used and a concentration thereof, a kind of a precipitant added and a concentration thereof, protein concentration, salt concentration, temperature and the like can be involved. A method for controlling and investigating the factors includes batch methods, dialysis methods, vapor diffusion methods (hanging-drop method, sitting-drop method and the like) and the like, described, for instance, in Blundell, T. L. et al., *PROTEIN CRYSTALLOGRAPHY*, 59-82 (1976), published by Academic Press, or the like.

The method for crystallization includes the batch methods, dialysis methods, vapor diffusion methods and the like. By the above method, physical and chemical factors such as a hydrogen ion concentration (pH), a kind and a concentration of the buffer used, and a kind and a concentration of the precipitant used, and physical and chemical factors such as protein concentration, salt

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concentration and temperature can be also determined.

The hydrogen ion concentration (pH) can be adjusted with a buffer. It is desired that the buffer is a buffer having buffering action in a broad range of pH, and being capable of suppressing precipitation of a non-proteinous crystal between the co-existing ion in the solution used during crystallization and the precipitant or the like. The buffer includes Tris-hydrochloric acid buffer, phosphate buffer, cacodylate buffer, acetate buffer, citrate buffer, glycine buffer and the like.

The precipitant may be a substance capable of elevating an effective concentration of the protein or changing a hydrogen ion concentration (pH) of the protein solution. Generally, the precipitant includes salts such as ammonium sulfate, sodium sulfate, sodium phosphate, potassium phosphate, sodium citrate, ammonium citrate, sodium chloride, potassium chloride and ammonium chloride; polyethylene glycols having various average molecular weights of about 200, about 1000, about 2000, about 4000, about 6000, about 8000, about 20000 or the like; organic solvents such as 2-methyl-2,4-pentadiol, methanol, ethanol, isopropanol, butanol and acetone, and the like.

The protein concentration may be a concentration suitable for crystallization, and it is desired that the protein concentration is, for example, 1 to 50 mg/ml, preferably 5 to 20 mg/ml, more preferably 7 to 15 mg/ml.

It is desired that the temperature conditions are 3° to 25°C, preferably 12° to 22°C.

In the case where the crystallization is carried out by the batch method, the crystallization can be carried out by gradually adding a precipitant solution comprising a precipitant, buffer and the like, so as to form a layer on the top layer of the solution containing the dipeptidyl peptidase IV to give a mixture, or by gradually adding the solution comprising the dipeptidyl peptidase IV, so that the solution is an upper layer of the precipitant solution to give a mixture. Here, the mixture is allowed to stand in a tightly closed vessel.

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In the case where the crystallization is carried out by the dialysis method, the crystallization can be carried out by placing a solution comprising dipeptidyl peptidase IV in a size exclusion semi-permeable membrane, and placing a precipitant solution outside of the size exclusion semi-permeable membrane as a reservoir solution, thereby diffusing the reservoir solution to the solution comprising the dipeptidyl peptidase IV via the semi-permeable membrane.

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In the case where the crystallization is carried out by the hanging-drop method in the vapor diffusion method, the crystallization can be carried out by placing a mixed solution of a solution comprising the dipeptidyl peptidase IV and a precipitant solution in a closed vessel allowing to be hanged at a position above the upper space of a reservoir in which the precipitant solution is contained as a reservoir solution, wherein the vapor pressure of the reservoir solution in the reservoir is set to be lower than that of the mixed solution.

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In the case where the crystallization is carried out by the sitting-drop method in the vapor diffusion method, the crystallization can be carried out by placing a mixed solution comprising a solution comprising the dipeptidyl peptidase IV and a precipitant solution in a closed vessel at a position higher than the liquid surface of a reservoir in which the precipitant solution is contained as a reservoir solution, wherein the vapor pressure of the reservoir solution in the reservoir is set to be lower than that of the mixed solution.

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The crystallization can be carried out by the sitting-drop method from the

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viewpoint of obtaining excellent-quality and large crystal.

When the obtained crystal is a crystal insufficient to ensure the X-ray structural analysis, the crystal may be grown by a seeding method such as macroseeding method or micro-seeding method, using the obtained crystal as a seed crystal.

When the macro-seeding method is performed, it is desired that the seed crystal is a single crystal that can be isolated by procedures under microscope wherein the seed crystal has excellent external form (having excellent crystallinity). Also, it is desired that the seed crystal is washed with a drop of a solution obtained by diluting the precipitant, for example, by 0.5 to 1.0-fold. It is desired that the solution used for seeding of the seed crystal is a protein solution having a degree of supersaturation that the crystal grows but the crystal nuclei do not grow. On the other hand, when the micro-seeding method is performed, the form and size of the seed crystal are not particularly limited.

The sequence information for the dipeptidyl peptidase IV and cDNA encoding the dipeptidyl peptidase IV can be obtained from a known information source [GenBank/EMBL accession No: X60708; Misumi et al., *Biochim. Biophys. Acta*, 1131, 333-336, (1992); GenBank/EMBL accession No: M80536; Darmoul et al., *J. Biol. Chem.*, 267, 4824-4833, (1992)]. Therefore, the dipeptidyl peptidase IV or a soluble polypeptide thereof can be produced by using conventional means for gene engineering on the basis of the above sequence information.

The nucleic acid used for production of the dipeptidyl peptidase IV or a soluble polypeptide thereof may be any nucleic acid in which the encoded polypeptide exhibits a dipeptidyl peptidase IV activity. For example, a nucleic

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acid encoding a polypeptide consisting of the amino acid sequence in which a transmembrane region in the N-terminal side (a region containing at least the amino acid nos: 1-28, preferably the region of the amino acid nos: 1-32) is deleted from the full-length human dipeptidyl peptidase IV, and a tag peptide is optionally added to a C-terminal side or N-terminal side of the amino acid sequence.

The nucleic acid can be obtained by, for instance, obtaining a fragment comprising a nucleic acid encoding a full-length dipeptidyl peptidase IV or a part thereof by means of conventional DNA recombination technique, and appropriately arranging the obtained fragment.

SEQ ID NO: 1 shows a sequence of a nucleic acid encoding a full-length dipeptidyl peptidase IV of human colon.

The nucleic acid (DNA or RNA) encoding a full-length dipeptidyl peptidase IV includes, for instance, a nucleic acid comprising human nucleic acids comprising the nucleotide sequence of SEQ ID NO: 1 without being limited thereto, and includes its naturally occurring variant, artificially modified variant, a homolog or ortholog derived from heterogeneous organism.

In other words, besides the nucleic acid comprising the nucleotide sequence of SEQ ID NO: 1, the nucleic acid includes a nucleic acid capable of hybridizing with a nucleic acid comprising the nucleotide sequence of SEQ ID NO: 1 under stringent conditions, more preferably under high-stringent conditions), or a complement thereof (nucleic acid having a complementary sequence).

Concrete examples of the nucleic acid described above include, for instance, a nucleic acid having usually about 70% or more, preferably about 80%

or more, more preferably about 85% or more, still more preferably about 90% or more, still more preferably about 95% or more, homology to the nucleotide sequence of SEQ ID NO: 1, and it is preferable that the polypeptide encoded by the above nucleic acid has a dipeptidyl peptidase IV activity.

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The dipeptidyl peptidase IV activity can be measured by, for example, incubating in a 1.5 ml reaction mixture [composition: 1.5 mM substrate (Gly-Pro-paranitroanilide), 71 mM glycine-NaOH (pH 8.7)] at 37°C for 10 minutes, and determining the liberated paranitroanilide at the absorbance of 405 nm. One unit (1 U) of a dipeptidyl peptidase IV is defined as an amount of the enzyme required for liberating 1 µmol of paranitroanilide per 1 minute.

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In the present invention, the hybridization under stringent conditions can be carried out as normal stringent conditions by performing hybridization in a hybridization solution having a salt concentration of $6 \times SSC$ or an equivalent concentration thereto, under the temperature conditions of 50° to $70^{\circ}C$ for about 16 hours, and optionally performing pre-washing with a solution having a salt concentration of $6 \times SSC$ or an equivalent concentration thereto, and thereafter performing washing with a solution having a salt concentration of $1 \times SSC$ or an equivalent concentration thereof. Furthermore, as the conditions having still higher stringency (high-stringent conditions), the hybridization can be carried out by washing with a solution having a salt concentration of $0.1 \times SSC$ or an equivalent concentration thereto in the above method.

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The dipeptidyl peptidase IV used for the crystallization has purity that can form a crystal, and the purity can be confirmed by conventional means of confirming purity (for example, a method comprising electrophoresing a fraction by polyacrylamide gel electrophoresis, SDS-polyacrylamide gel electrophoresis

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or the like, and visualizing the fraction by silver staining, or the like).

The X-ray structural analysis data of the crystal can be obtained by subjecting the crystal of the present invention to an X-ray crystallographic structural analysis known to one of ordinary skill in the art [for example, see Blundell, T. L. et al., PROTEIN CRYSTALLOGRAPHY, 59-82 (1976), published by Academic Press, and the like, whereby a three-dimensional structural coordinate (a value showing the relationship of the spatial positions of each atom) and a three-dimensional structure model for the crystal can be obtained. Concretely, the three-dimensional structural coordinate of the dipeptidyl peptidase IV is obtained as an atomic coordinate by procedures comprising the steps of 1) irradiating the crystal of the present invention with a monochromatic X-ray to give an X-ray diffraction pattern, 2) obtaining X-ray diffraction intensity data from the X-ray diffraction pattern, 3) obtaining an electron density map by Fourier transform, and 4) allocating a polypeptide chain and side chain thereof on the electron density map based on the amino acid sequence of the polypeptide used for the crystal. Furthermore, the three-dimensional structure is clarified by molecule-modeling based on the three-dimensional structural coordinate. Therefore, the three-dimensional structural coordinate of the dipeptidyl peptidase IV obtained from the crystal of the present invention is also encompassed within the scope of the present invention.

The crystallographic parameters for the crystal are obtained from the X-ray diffraction intensity data of the crystal of the present invention. The crystal of the present invention is an orthorhombic crystal having a space group of $P2_12_12_1$, and a lattice constant of the unit cell of $|a| = 118.0 \pm 5.0$ Å, $|b| = 125.9 \pm 5.0$ Å, $|c| = 136.8 \pm 5.0$ Å, and $\alpha = \beta = \gamma = 90^{\circ}$. The crystal has a

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2.6Å resolution by X-ray crystallographic structural analysis, that is, the crystal has characteristics sufficient to ensure a resolution capable of analyzing up to the side chain level of the polypeptide.

It is a known fact to one of ordinary skill in the art that the same protein can be crystallized even under different conditions. Therefore, the present invention is not limited to only the conditions for crystallization, and the crystal that shows substantially the same crystallographic constants as those in the present invention are also encompassed within the scope of the present invention.

More concretely, the crystal of the dipeptidyl peptidase IV of the present invention has a structural coordinate as shown in Figure 4, or a structural coordinate different from the structural coordinate as shown in Figure 4 via fluctuation of a protein.

The crystal according to the present invention can also be used as a seed crystal for carrying out the crystallization of a polypeptide having a three-dimensional structure similar to that of the dipeptidyl peptidase IV used for, for example, carrying out the crystallization of the dipeptidyl peptidase IV, dipeptidyl peptidase IV-like proteins, homolog proteins and the like, which are derived from other organism species.

When the crystal of the present invention is irradiated with X-ray, a low-temperature measurement may be carried out, as described in Examples set forth below.

The X-ray structural analysis data are converted to a structure factor by evaluating the intensity of X-ray diffraction using MOSFILM Program Package (Version 6.1). Also, in order to obtain the information for the phase, multiple isomorphous replacement method or the like can be performed, for example, as

described in Examples.

In the structural analysis, CCP4 (Collaborative Computational Project, Number 4, 1994, "The CCP4 Suite: Programs for Protein Crystallography," Acta Cryst. D50, 760-763) program or the like is used.

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The three-dimensional structural coordinate of the dipeptidyl peptidase IV of the present invention can be obtained, for example, as follows. Firstly, Fourier transform calculation is carried out using the differences between the diffraction intensity obtained from two kinds of isomorphous replacement crystals of mercury and the diffraction intensity obtained from native crystal, and investigating the large peaks provided by the heavy atoms (mercury) on the Patterson's diagram to determine the locations of each mercury atoms in the unit cell of the real space. The phase of the crystal structure factor for the native crystal is determined using the obtained location coordinate for the mercury atoms. Furthermore, refinement is performed using the crystal structure factor of the native crystal and two kinds of the crystal structure factors of the isomorphous replacement crystals of mercury, and the coordinate for each of the mercury atoms is more accurately determined. An electron density map for the crystal of the dipeptidyl peptidase IV in the real space is obtained using the phase of the crystal structure factor of the native crystal calculated from the refined mercury atoms coordinate. Furthermore, the electron density map is improved by performing smoothing and histogram matching for the electron density map of the solvent region, whereby an electron density map necessary and sufficient for building a molecular model can be obtained. Next, the sites corresponding to the amino acid residues of the dipeptidyl peptidase IV on the electron density map are identified using QUANTA (manufactured by Accelrys, Inc.) to build the

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molecular model to give a three-dimensional structural coordinate.

The three-dimensional structural coordinate of the dipeptidyl peptidase IV of the present invention is shown in Figure 4. Figure 4 shows the obtained three-dimensional structural coordinates, according to the format of the Protein Data Bank, which is a notation generally used by one of ordinary skill in the art.

The three-dimensional structural coordinates shown in Figure 4 are those represented using the origin of the unit cell of the crystal as the origin of the three-dimensional space. The R factor that is considered as an index for the accuracy of the obtained molecular model is 24.89%, and the free R factor is 30.15%. In addition, the deviation in the interatomic bond distance from the ideal state of the three-dimensional structure (rms-deviation) and the deviation in the bond angle are 0.006Å and 1.305°, respectively. In the case, for instance, the three-dimensional structural coordinate of the present invention is used for the calculation by a computer, a novel structural coordinate obtained as a result of the operation for mathematical transfer, such as translation, rotation, or symmetry in the three-dimensional space without changing the relative configuration of the atoms, is also encompassed within the scope of the present invention. Furthermore, not only all of the three-dimensional structural coordinate of the present invention but also a part thereof are also encompassed within the scope of the present invention.

The three-dimensional structural coordinate of the dipeptidyl peptidase IV of the present invention can be used, for example, as shown in Figure 3, for three-dimensional graphic displaying of the stereogram of the three-dimensional structure model, and for evaluation of the structure-activity relationship and the quantitative structure-activity relationship. Also, the structural features of the

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crystal of the present invention can be more concretely shown using the threedimensional structural coordinate shown in Figure 4. The evaluation of the structure-activity relationship or quantitative structure-activity relationship by the three-dimensional structure model is also encompassed within the scope of the present invention.

According to the three-dimensional structural coordinate of the dipeptidyl peptidase IV of the present invention, one of the characteristics of the dipeptidyl peptidase IV can be found in that the dipeptidyl peptidase IV has 273 molecules of bond water in an asymmetric unit and has 5 molecules of N-acetylglucosamine residues per 1 molecule of the dipeptidyl peptidase IV.

According to the three-dimensional structural coordinate of the dipeptidyl peptidase IV of the present invention, the information for atoms or atomic groups of the side chain of the dipeptidyl peptidase IV, interacting with the atoms or atomic groups of a known effector of the dipeptidyl peptidase IV via an intermolecular interaction can be obtained.

Furthermore, according to the three-dimensional structural coordinate of the dipeptidyl peptidase IV of the present invention, the information of regions in the dipeptidyl peptidase IV that are susceptible to binding or intermolecular interaction with the effector can be obtained.

In addition, according to the three-dimensional structural coordinate of the dipeptidyl peptidase IV of the present invention, the information of the structure specific to the dipeptidyl peptidase IV, which is not found in proteins other than the dipeptidyl peptidase IV, can be obtained. Therefore, higher selectivity in the effector targeting a protein other than the dipeptidyl peptidase IV can be designed, when the effector also acts on the dipeptidyl peptidase IV.

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The intermolecular interaction includes covalent bond, ionic interaction, ion-dipole interaction, dipole-dipole interaction, hydrogen bonding, van der Waals force, electrostatic interaction, hydrophobic interaction and the like.

In the present specification, the atoms or atomic groups of the effector and atoms or atomic groups of the side chain of the dipeptidyl peptidase IV, which interact with each other via intermolecular interaction, are referred to as "pharmacophore."

Also, according to the three-dimensional structural coordinate of the dipeptidyl peptidase IV of the present invention, the information for the structure specific for the dipeptidyl peptidase IV, which is not found in proteins other than the dipeptidyl peptidase IV, can be provided.

In addition, for example, when the measurement conditions are different in X-ray diffraction, or the three-dimensional structure of the complex in the solution is analyzed using multidimensional NMR, and the like, the three-dimensional structural coordinate may differ from that shown in Figure 4. The three-dimensional structural coordinate varies depending on the fluctuation of protein and the like, and is encompassed within the scope of the present invention.

In the present specification, the "fluctuation of protein" means a state that is caused by molecular oscillation, temperature and the like, and accompanied with the structural change that can exhibit an activity for the dipeptidyl peptidase IV in a living body.

Also, according to the three-dimensional structural coordinate of the dipeptidyl peptidase IV of the present invention, one of the characteristics of the dipeptidyl peptidase IV resides in that the amino acid residues, Ser 630, Asp 708

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and His 740, which are involved in the activity deduced by experiments by using various active inhibitors of the dipeptidyl peptidase IV, exist in the adjacent area, even though the amino acid residues exist in distant locations on the primary sequence. Concretely, the distance between the $O_{\delta 2}$ atom of Asp 708 and the $N_{\delta 1}$ atom of His 740, and the distance between the $N_{\epsilon 2}$ atom of His 740 and the O_{γ} atom of Ser 630 are distances that can form hydrogen bonding.

Therefore, the present invention also includes a three-dimensional structural coordinate of the region in the dipeptidyl peptidase IV, which is involved in binding or interaction of the dipeptidyl peptidase IV with an effector thereof, including a three-dimensional structural coordinate of a region selected from the group consisting of the following (a) to (d):

- (a) a region characterized by Ser 630, Asp 708 and His 740 in the amino acid sequence of SEQ ID NO: 2, and all or a part of a group of amino acid residues located in the adjacent area of each of the Ser 630, Asp 708 and His 740 in the structural coordinate shown in Figure 4 or the three-dimensional structure model defined by the structural coordinate;
- (b) a region characterized by Ser 630, Asp 708 and His 740 in the amino acid sequence of SEQ ID NO: 2, and

 20 all or a part of a group of amino acid residues comprising amino acids capable of maintaining physicochemical characteristics physiologically equivalent to each of amino acids of the group of amino acid residues located in the adjacent area of each of Ser 630, Asp 708 and His 740, in the structural coordinate shown in Figure 4 or the three-dimensional structure model defined by the structural coordinate,

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- aregion characterized by a group of amino acid residues comprising amino acids capable of maintaining physicochemical characteristics physiologically equivalent to each of Ser 630, Asp 708 and His 740 in the amino acid sequence of SEQ ID NO: 2, and all or a part of a group of amino acid residues located in the adjacent area of said group of the amino acid residue in the structural coordinate shown in Figure 4 or the three-dimensional structure model defined by the structural coordinate; and
- (d) a region characterized by a group of amino acid residues comprising

 amino acids capable of maintaining physicochemical characteristics

 physiologically equivalent to each of Ser 630, Asp 708 and His 740 in the

 amino acid sequence of SEQ ID NO: 2, and

all or a part of a group of amino acid residues of a group of amino acid residues comprising amino acids capable of maintaining physicochemical characteristics physiologically equivalent to the each amino acid of the amino acid residues located in the adjacent area of said groups of the amino acids, in the structural coordinate shown in Figure 4 or the three-dimensional structure model defined by the structural coordinate.

In the present specification, the "adjacent (area)" refers to an area involved in covalent bond, ionic interaction, ion-dipole interaction, dipole-dipole interaction, hydrogen bonding, van der Waals force, electrostatic interaction, hydrophobic interaction or the like with the amino acid residues, concretely, a region within 10Å, preferably within 8Å, more preferably within 5Å.

The physicochemical characteristic includes features in shape of the three-dimensional structure, hydrophobicity, electric charge, pK and the like.

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The "amino acid capable of maintaining physicochemical characteristics physiologically equivalent" may be an amino acid analogue residue obtained by replacing a side chain of amino acid residues in the three-dimensional structural coordinate shown in Figure 4 with other side chain, for example, showing bioisosterism. Alternatively, the amino acid residue in the three-dimensional structural coordinate shown in Figure 4, may be replaced with another amino acid residue belonging to the same Group, in any of the following Groups I to VI:

- I glycine, alanine;
- 10 II valine, isoleucine, leucine;
 - III aspartic acid, glutamic acid, asparagine, glutamine;
 - IV serine, threonine;
 - V lysine, arginine;
 - VI phenylalanine, tyrosine.

According to the three-dimensional structural coordinate of the dipeptidyl peptidase IV of the present invention, a three-dimensional structural coordinate of a polypeptide can be easily derived if an accurate amino acid sequence is determined, even when the polypeptide is a dipeptidyl peptidase IV or a dipeptidyl peptidase IV-like protein derived from other organism species, as long as the polypeptide is a polypeptide having high homology on the level of amino acid sequence with the dipeptidyl peptidase IV used for the preparation of the crystal of the present invention (for example, at least 20%, preferably 30% or more, more preferably 40% or more).

Furthermore, the three-dimensional structural coordinate of the dipeptidyl peptidase IV of the present invention can be used for X-ray crystallographic

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structural analysis of the crystal and the like of other proteins having an amino acid sequence with significant homology with the dipeptidyl peptidase IV used for the preparation of the crystal of the present invention. Concretely, according to the molecular replacement method [for example, see Blundell, T. L. et al., PROTEIN CRYSTALLOGRAPHY, 446-464 (1976), published by Academic Press and the like], the three-dimensional structural coordinate thereof can be quickly and readily obtained from the structure factors obtained by the X-ray diffraction pattern of the crystal, without using multiple isomorphous replacement method, even for the determination of the structural coordinate of the above-mentioned crystal of which structural coordinate has not yet been known.

In the present specification, the term "significant homology" is a case where there is identity of 20%, or more, preferably by 30% or more, between the amino acid sequences.

When the molecular replacement method is performed, for example, a program such as X-PLOR and CNX (both manufactured by Accelrys Inc.) or AMORE [one of the programs of CCP4 (Collaborative Computational Project, Number 4), *Acta Crystallogr.* **D50**, 670-673 (1994)] can be run by a computer on which the program can be executed. Here, whether or not the molecular replacement method is applicable can be determined by actually applying the molecular replacement method to the structure factors calculated from the X-ray diffraction pattern of the desired crystal and obtaining a significant solution.

In other words, the three-dimensional structural coordinate obtained by structural analysis by molecular replacement method is encompassed within the scope of the present invention as long as a significant solution is obtained. The present invention also encompasses a three-dimensional structural coordinate of

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a dipeptidyl peptidase IV, or a dipeptidyl peptidase IV-like protein, namely a homolog protein or the like of other organism species derived by the above method.

Therefore, according to the present invention, a method for obtaining a three-dimensional structural coordinate of a homolog protein of a dipeptidyl peptidase IV comprising the step of performing refinement of an electron density map of the homolog protein of the dipeptidyl peptidase IV comprising the amino acid sequence of SEQ ID NO: 2, based on the three-dimensional structural coordinate of the present invention, to give a three-dimensional structural coordinate is provided. Also, a method for obtaining a three-dimensional structural coordinate of a crystal of a complex of a dipeptidyl peptidase IV and an effector of the dipeptidyl peptidase IV, based on the three-dimensional structural coordinate of the present invention, is likewise provided.

According to the three-dimensional structural coordinate of the dipeptidyl peptidase IV of the present invention, a method for identifying a region or site for a target for binding or interaction between the dipeptidyl peptidase IV and an effector of the dipeptidyl peptidase IV is provided, based on the analysis of the binding regions between the dipeptidyl peptidase IV and a known effector of the dipeptidyl peptidase IV such as an inhibitor, or based on the simulation of the interaction between the dipeptidyl peptidase IV and a known effector of the dipeptidyl peptidase IV.

Also, based on the three-dimensional structural coordinate of the dipeptidyl peptidase IV of the present invention and the steric conformation of the effector of the dipeptidyl peptidase IV, the pharmacophore of the effector of the dipeptidyl peptidase IV can be identified. A method for identifying the

pharmacophore is also provided. The method is useful for designing an effector having excellent characteristics such as higher avidity, higher biological activity, higher biological stability, higher thermodynamic stability, higher absorbency to a living body, and lower toxicity.

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Concretely, for example, the region or site for a target involved in binding or interaction of the dipeptidyl peptidase IV and an effector of the dipeptidyl peptidase IV, can be identified by:

- 1) obtaining a crystal of a complex of the dipeptidyl peptidase IV and a known effector of the dipeptidyl peptidase IV such as an inhibitor, and obtaining a three-dimensional structural coordinate of the crystal based on the three-dimensional structural coordinate of the dipeptidyl peptidase IV of the present invention and the steric conformation of the effector of the dipeptidyl peptidase IV, whereby obtaining the three-dimensional structural coordinate of a binding region of the dipeptidyl peptidase IV and the effector;
- 2) simulating an intermolecular interaction between the dipeptidyl peptidase IV and a known effector of the dipeptidyl peptidase IV based on the three-dimensional structural coordinate of the dipeptidyl peptidase IV of the present invention and the steric conformation of the effector of the dipeptidyl peptidase IV;

or the like.

The crystal of the above-mentioned complex can be obtained by, for example, incubating the crystal of the present invention in a solution comprising the effector, forming a complex of the dipeptidyl peptidase IV and the effector, and crystallizing the obtained complex, and the like.

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Also, when the three-dimensional structural coordinate of the crystal of

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the complex is obtained, the steric structure of the effector of the abovementioned complex can be readily obtained by calculating the differential Fourier diagram utilizing a three-dimensional structure model defined by the three-dimensional structural coordinate of the dipeptidyl peptidase IV of the present invention, whereby specific interaction forms and interaction sites between the dipeptidyl peptidase IV and the effector can be readily clarified.

When the intermolecular interaction is simulated, for example, the space regions, residues and the like in which covalent bond, ionic interaction, ion-dipole interaction, dipole-dipole interaction, hydrogen bonding, van der Waals force, electrostatic interaction, hydrophobic interaction or the like can be simulated, based on the three-dimensional structural coordinate of the dipeptidyl peptidase IV of the present invention and the steric conformation of the effector of the dipeptidyl peptidase IV.

Furthermore, according to the three-dimensional structural coordinate of the dipeptidyl peptidase IV of the present invention, the three-dimensional structural coordinate or the three-dimensional structure model based on the three-dimensional structural coordinate regarded as an active center of the dipeptidyl peptidase IV, sites indirectly acting on the active center and regions or sites involved in binding or interaction with the effector, or the like, is obtained, whereby a compound capable of specifically acting on the dipeptidyl peptidase IV can be designed, identified, evaluated or searched.

For example, in the structural coordinate of Figure 4 and the threedimensional structure model defined by the structural coordinate, a compound capable of modifying the activity of the dipeptidyl peptidase IV can be designed, identified, evaluated or searched, based on the regions characterized by Ser 630,

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Asp 708 and His 740, and all or a part of amino acid residues of the group of the amino acid residues located in the adjacent area of the Ser 630, Asp 708 and His 740.

Therefore, according to the present invention, a method for designing, identifying, evaluating or searching an effector of the dipeptidyl peptidase IV is provided.

One of the significant features of the method of the present invention for designing, identifying, evaluating or searching an effector resides in that the method comprises designing, identifying, evaluating or searching a compound capable of acting on the dipeptidyl peptidase IV, based on the three-dimensional structural coordinate of the present invention.

According to the method of the present invention for designing, identifying, evaluating or searching an effector, since the method is based on the three-dimensional structural coordinate of the dipeptidyl peptidase IV of the present invention, the information for a structure specific to the dipeptidyl peptidase IV, which is not found in proteins other than the dipeptidyl peptidase IV can be obtained. Therefore, according to the method of the present invention for designing, identifying, evaluating or searching an effector, the method has an excellent effect that the selectivity of the effector of the dipeptidyl peptidase IV can be enhanced.

Also, according to the method of the present invention for designing, identifying, evaluating or searching an effector, since the method is based on the three-dimensional structural coordinate of the dipeptidyl peptidase IV of the present invention, visual studies and/or energy calculation can be made according to the method by using a computer and the like. Therefore, there are

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exhibited some excellent effects that a compound having excellent characteristics such as having higher avidity, higher biological activity, higher biological stability, higher thermodynamic stability, higher absorbency in a living body, and lower toxicity, than those for a known inhibitor can be designed, identified, evaluated or searched, and that logical design can be performed in the three-dimensional space.

In the present specification, the "effector" includes a compound that inhibits or enhances the activity (i.e. inhibitor or activator), which may be natural compounds or synthetic compounds, or may be polymers or low-molecular weight compounds.

A concrete example of the method of the present invention for designing, identifying, evaluating or searching an effector includes a method comprising the steps of:

- (i) identifying a region to be targeted for binding or interaction with the effector in a dipeptidyl peptidase IV, based on all and/or a part of the three-dimensional structural coordinate of the present invention and the steric conformation of the effector of the dipeptidyl peptidase IV;
- (ii) identifying corresponding atoms or atomic groups capable of generating in the region at least one intermolecular interaction selected from the group consisting of covalent bond, ionic interaction, ion-dipole interaction, dipole-dipole interaction, hydrogen bonding, van der Waals force, electrostatic interaction and hydrophobic interaction, with the atoms or atomic groups existing in a candidate compound; and
- (iii) designing a compound based on the above information of the above step(i) and/or (ii).

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The three-dimensional structural coordinate used for designing, identifying, evaluating or searching a compound capable of binding to the dipeptidyl peptidase IV may be a coordinate fixed in the three-dimensional space, and the intensity of binding with the compound or the like can be calculated by carrying out translation or rotation in the three-dimensional space, and transfer to an extent that the chemical covalent bond would not be cleaved in the amino acid residues of the dipeptidyl peptidase IV.

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In the above step (i), the "region to be targeted in the dipeptidyl peptidase IV" preferably includes an active center of the dipeptidyl peptidase IV, sites indirectly acting on the active center and the like. For example, there is included a region characterized by Ser 630, Asp 708 and His 740 and all or a part of a group of the amino acid residues located in the adjacent area of Ser 630, Asp 708 and His 740, and the like in the structural coordinate of Figure 4 and the three-dimensional structure model defined by the structural coordinate. The atoms or atomic groups that can be matched therewith are identified, based on the three-dimensional structural coordinate of an active center, sites indirectly acting on the active center and the like, whereby the candidate atoms or candidate atomic groups can be obtained.

In the above step (ii), for example, the atoms or atomic groups capable of associating via intermolecular interaction between the atoms or atomic groups in the region, concretely, the corresponding atoms or atomic groups capable of generating covalent bond, ionic interaction, ion-dipole interaction, dipole-dipole interaction, hydrogen bonding, van der Waals force, electrostatic interaction, hydrophobic interaction and the like, are searched and extracted, based on the information identified in the above step (i).

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Next, in the above step (iii), the corresponding atoms or atomic groups searched in the above step (i) and/or (ii) are combined to design a compound.

Thereafter, if desired, whether or not the compound designed in the above step (iii) is matched via intermolecular interaction with the side chains and atoms or atomic groups in the dipeptidyl peptidase IV as defined by the three-dimensional structural coordinate of the present invention can be simulated.

The compound designed, identified, evaluated or searched by the above steps (hereinafter also referred to as a candidate compound in the present specification) can be obtained by generally used chemical synthetic methods, depending on the compound.

In addition, in the method of the present invention for designing, identifying, evaluating or searching an effector, there can be carried out a step of detecting the interaction between the dipeptidyl peptidase IV and the candidate compound. When the interaction is detected, the interaction serves as an index showing that the above candidate compound is a compound capable of binding to the dipeptidyl peptidase IV.

The above interaction can be detected by, for example, plasmon resonance analysis apparatus, mass spectrometer, titration isothermal calorimetry, NMR and the like. For example, in the case of plasmon resonance analysis apparatus, when a sensorgram indicates the formation of a complex, by contacting the dipeptidyl peptidase IV-immobilized matrix with the candidate compound and performing analysis by optical detection (for example, photometer, polarization photometer and the like) and the like, it would be an index showing that the interaction between the candidate compound and the dipeptidyl peptidase IV is generated. For example, in the case of a mass spectrometer, when a spectrum

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indicates the formation of a complex, by contacting the dipeptidyl peptidase IVimmobilized matrix with the candidate compound and performing analysis with a mass spectrometer (matrix-assisted laser desorption/ionization-time of flight mass spectrometry: MALDI-TOF MS, electro spray-ionization mass spectrometer: ESI-MS and the like), it would be an index showing that the interaction between the candidate compound and the dipeptidyl peptidase IV is generated. For example, in the case of titration-thermal calorimetry interaction analysis, when the titration curve indicates the formation of a complex, by contacting a solution of the dipeptidyl peptidase IV with the candidate compound, and measuring the heat coming in and out of a thermal diode and the like, it would be an index showing that the interaction between the candidate compound and dipeptidyl peptidase IV is generated. For example, in the case of NMR, when a spectrum indicates the formation of a complex, by analyzing by NMR a solution prepared mixing the dipeptidyl peptidase IV and a candidate compound, it would be an index showing that the interaction between the candidate compound and the dipeptidyl peptidase IV is generated.

Furthermore, the method of the present invention for designing, identifying, evaluating or searching an effector may further comprise the steps of contacting the dipeptidyl peptidase IV with a candidate compound, and thereafter measuring the activity of the dipeptidyl peptidase IV. When the dipeptidyl peptidase IV activity increases or decreases, it would be an index showing that the candidate compound is a compound having enhancing action or inhibitory action on the activity of the dipeptidyl peptidase IV.

The dipeptidyl peptidase IV activity can be measured by, for example, incubating a 1.5 ml reaction mixture [composition: 1.5 mM substrate

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(Gly-Pro-paranitroanilide), 71 mM glycine-NaOH (pH 8.7)] at 37°C for 10 minutes in the presence of a candidate compound, and measuring the liberated paranitroanilide at the absorbance of 405 nm. During the measurement of the activity, the candidate compound may be evaluated by using a reaction system in which a suitable dilution series of the compound is added thereto.

The method of the present invention for designing, identifying, evaluating or searching the effector can be performed by, for example, sequentially selecting the interaction between the dipeptidyl peptidase IV and the compounds in a database in a computer to which the structures of plural of compounds had been inputted, or the interaction between the dipeptidyl peptidase IV and the designed compound, by visual methods (visual selection method) utilizing the database; and/or sequentially calculating the avidity with a computer, and searching a compound capable of stably interacting with the dipeptidyl peptidase IV from the database (computer-assisted avidity evaluation method) and the like, based on the three-dimensional structural coordinate of the present invention.

In the above visual selection method, the database of the structures of compounds may be a database in which the three-dimensional structural coordinates have been determined and inputted. Alternatively, in the case of a compound having a low molecular weight, the database may be a database in which the information for chemical covalent bond of a compound having a low molecular weight had been inputted, because the conformation can be relatively freely changed, and the three-dimensional structural coordinate of each conformation can be derived by calculation in a relatively short time.

Concretely, in the visual selection method, the expected complex between the dipeptidyl peptidase IV and a candidate compound or a part thereof is firstly

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displayed on a computer screen, based on the three-dimensional structural coordinate of the present invention. Next, the intermolecular interaction binding between a compound in the database and the binding regions of the dipeptidyl peptidase IV is simulated on the computer, taking chemical interaction into consideration. Also, the simulation of the chemical modification of the compound is performed on the computer, and the changes in the interaction caused as a result thereof are observed on the computer screen. During the simulation, the three-dimensional space can be more easily understood by displaying the three-dimensional structure of the protein on the computer screen so that the structure corresponds to Crystal Eye glasses supplied by Silicone Graphics; simultaneously displaying two screens in which each angle is adjusted for displaying the object, according to the visual fields of the right eye and left eye, which is so-called referred to as "stereovision" which is frequently used by one of ordinary skill in the art; or the like. In addition, the three-dimensional structure can be visually studied by methods other than the stereoscopic displaying of the three-dimensional structure.

The candidate compound capable of generating suitable interaction can be obtained by displaying on a computer a group of candidates with appropriate conformation and selecting an appropriate one therefrom; calculating a structure having a low energy state on a computer; or the like. Next, a derivative of a compound capable of generating more preferable binding with the dipeptidyl peptidase IV may be searched among the candidate compound.

More specifically, on the level of the three-dimensional structure, the followings may be taken into consideration:

25 a group likely to be charged negatively, such as carboxyl group, nitro

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group, or a halogen group in the compound interacts with an amino acid residue having a positive charge, such as lysine, arginine or histidine in the dipeptidyl peptidase IV;

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- a group likely to be charged positively, such as amino group, imino group 2 or guanidyl group in the compound interacts with an amino acid residue having negative charge, such as glutamic acid or aspartic acid in the dipeptidyl peptidase IV;
- 3 a hydrophobic functional group such as an aliphatic group or an aromatic group in the compound interacts with a hydrophobic amino acid residue such as alanine, leucine, isoleucine, valine, proline, phenylalanine, tryptophane or methionine in the dipeptidyl peptidase IV;
- a group involved in hydrogen bonding, such as hydroxyl group or amide 4 group is allowed to form hydrogen bonding with a main chain or side chain portion;
- 5 a group or an atom likely to be charged negatively, such as carboxyl group, 15 nitro group or a halogen group in the compound interacts with a positively charged atom on a main chain or side chain portion;
 - 6 a group or an atom likely to be charged positively, such as amino group. imino group or guanidyl group in the compound interacts with a negative charged atom on a main chain or a side chain portion;
 - 7 the flexibility of the three-dimensional structure of the compound is lowered by, for instance, cyclizing the linear chain portion:

or the like. For example, a derivative may be designed and synthesized so that the atoms having negative charge of the candidate compound are located in the adjacent region of the side chain of an amino acid residue having positive charge

such as lysine, arginine or histidine, in the amino acid residue of the dipeptidyl peptidase IV, and that an atom having positive charge of the candidate compound is located in the adjacent region of the side chain of the amino acid residue having negative charge such as glutamic acid or aspartic acid in the amino acid residue of the dipeptidyl peptidase IV. Also, a group suitable for forming a hydrophobic interaction may be introduced into the portion capable of forming a hydrophobic interaction between the compound and the dipeptidyl peptidase IV, to design and synthesize a derivative. In addition, a group suitable for forming hydrogen bonding may be introduced into the portion capable of forming hydrogen bonding between the compound and the dipeptidyl peptidase IV, to design and synthesize a derivative. In the above-mentioned designing, it is desirable that van der Waals interaction is as high as possible, and that steric hindrance does not occur between each of the atoms. Furthermore, it is desirable that new void portions are not produced by modification of the compound and that in regions already containing void portions, the void portions are filled as much as possible.

As described above, the design, identification, evaluation or searching of a final compound can be thus performed with visually comprehensively considering intermolecular interaction and other factors on a computer screen.

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In the computer-assisted avidity evaluation method, in order to determine the validity for the designing of a new compound, and to obtain a compound that can stably interact from the compounds in the database, a docking software (DOCK, GOLD, FlexX, Glide or the like) is used for evaluation of binding based on the energy by calculating a molecular force field between the compound and the dipeptidyl peptidase IV, evaluation of binding based on chemical

characteristics, evaluation of binding based on the Protein Data Bank (PDB), and the like. Further, in a model system consisting of the compound and the dipeptidyl peptidase IV, or in a model system further comprising solvent molecules and the like, it can be led to a compound that can stably interact by obtaining the index showing avidity, such as free energy of bonding, the ratio obtained from bond state number and non-bond state number, and the like by using molecular kinetic calculation or Monte Carlo calculation. The programs for calculation of molecular force field and molecular kinetic include AMBER, CHARMM, DISCOVER, PRESTO and the like, and the force field used includes AMBER, CHARMM, OPLS, MMCF, CVFF and the like. Furthermore, a program such as Ludi which automatically outputs the candidates for a candidate compound by providing a three-dimensional structural coordinate of the amino acid residues interacting in the dipeptidyl peptidase IV may be used.

The visual selection method and computer-assisted avidity evaluation method can be performed alone or in combination. In the case of performing the methods in combination, the avidity is actually calculated for the compounds that has been expected to be more desirable in visual investigation, and the validity thereof is evaluated. By repeatedly performing the calculation and evaluation, more excellent compounds may be designed, identified, evaluated or searched.

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Next, the designed, identified, evaluated or searched compound is optimized to be a more excellent compound, such as a compound having more excellent characteristics as a medicament, such as being excellent *in vivo* kinetics, having low toxicity and low side-effect; a compound having a still higher biological activity as an effector; a compound having an advantageous structure as a medicament in view of its oral administration; and the like.

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The resulting candidate compound can be obtained using generally used techniques for chemical synthesis depending on the kind of the compound.

The present invention also encompasses an effector of the dipeptidyl peptidase IV, which is obtained by the method of the present invention for designing, identifying, evaluating or searching an effector. When the effector is a compound capable of inhibiting or enhancing the activity of the dipeptidyl peptidase IV, the effector (inhibitor or activator) is expected to be an agent for, for example, a modulatory agent of immune response, a therapeutic or prophylactic agent for diabetes, inflammation, multiple sclerosis, Graves' disease, chronic rheumatoid arthritis, AIDS, cancer and the like.

The three-dimensional structural coordinate of the dipeptidyl peptidase IV of the present invention can be provided as a computer program, a medium or the like, which displays the three-dimensional structure of the molecule based on the three-dimensional structural coordinate and can be provided via a telecommunication line or the like. Therefore, using a computer or the like, the three-dimensional coordinate of the dipeptidyl peptidase IV can be displayed in detail, allowing to perform the method of the present invention for designing, identifying, evaluating or searching an effector more rapidly, conveniently and logically.

The present invention also encompasses a program or a medium therefor for use of the three-dimensional structural coordinate, in which all and/or a part of the three-dimensional structural coordinate of the dipeptidyl peptidase IV of the present invention is recorded.

The medium may be any of those in which the three-dimensional structural coordinate of the present invention can be derived on a program that

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runs on a computer, and includes, for instance, electric memory media referred to as memory; semi-permanent memory media such as a FD, a hard disk, an optical disk, an opto-magnetic disk and a magnetic tape, and the like. In addition, the program and the medium therefor for use of the three-dimensional structural coordinate of the present invention also encompass those having a form which can be communicated via a telecommunication line such as internet.

Also, the program and the medium therefor for use of the three-dimensional structural coordinate of the present invention may further comprise a means for displaying the three-dimensional graphic display of the molecule. The program or the medium therefor which comprises the means for displaying the three-dimensional graphic display has advantages that visual studies and/or calculation of avidity can be made more conveniently, so that there is more facilitated a logical design on the three-dimensional structural level for obtaining a compound having excellent characteristics such as higher avidity, higher biological activity, higher biological stability, higher thermomechanical stability, higher absorbency to a living body, and lower toxicity than those for known effectors of the dipeptidyl peptidase IV.

As the means capable of displaying the three-dimensional graphic display, there may be generally used a program that is made so that a means for inputting the three-dimensional structural coordinate of the molecule, a means for measuring visual representation of the coordinate on a computer screen, the distance between the represented atoms in the molecule, bond angles or the like, a means for addition or modification of the coordinate, and the like can be provided. Furthermore, there may be used a program that has been made so that a means for calculating the structure energy of the molecule based on the

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coordinate of the molecule, a means for calculating the free energy of bonding, and the ratio of bonding state number to non-bonding state number in consideration of solvent molecules such as water molecule can be provided. Examples of the program suitable for such purposes include Insight II, QUANTA and the like, which are computer programs commercially available from Accelrys Inc., and the present invention is not limited to these programs. Also, the above-mentioned programs can be introduced into a computer referred to as a work station supplied from Silicone Graphics Inc., SunMicro-Systems Ltd., or the like, and used.

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According to the crystal of dipeptidyl peptidase IV of the present invention, there can be exhibited excellent effects that the three-dimensional structural coordinate can be obtained as an information for designing, identifying, evaluating or searching an effector of the dipeptidyl peptidase IV useful as a modulatory agent of immune response and as a therapeutic or prophylactic agent for diabetes, inflammation, multiple sclerosis, Graves' disease, chronic rheumatoid arthritis, AIDS, cancer and the like, and that the crystal of a complex of the dipeptidyl peptidase IV and a known effector can be readily prepared. Also, according to the three-dimensional structural coordinate of the present invention, there is exhibited an excellent effect that the effector can be designed, identified, evaluated or searched. In addition, according to the method for obtaining a three-dimensional structural coordinate of the homolog protein of the dipeptidyl peptidase IV of the present invention, there is exhibited an excellent effect that the three-dimensional structural coordinate of the homolog protein of the dipeptidyl peptidase IV of which three-dimensional structure is unknown can be conveniently and rapidly provided. Furthermore, according to the method for

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obtaining a three-dimensional structure of a crystal of a complex of the dipeptidyl peptidase IV of the present invention and an effector of the dipeptidyl peptidase IV, there is exhibited an excellent effect that the method can provide a target for designing an effector useful as a modulatory agent of immune response and as a therapeutic or prophylactic agent for diabetes, inflammation, multiple sclerosis, Graves' disease, chronic rheumatoid arthritis, AIDS, cancer and the like, and having excellent characteristics such as higher avidity, higher biological activity, higher biological stability, higher thermomechanical stability, and higher absorbency to a living body. Moreover, according to the method of the present invention for identifying a pharmacophore of the dipeptidyl peptidase IV and the effector of the dipeptidyl peptidase IV, there is exhibited an excellent effect that the method can provide a target for designing the effector useful as a modulatory agent of immune response and as a therapeutic or prophylactic agent for diabetes, inflammation, multiple sclerosis, Graves' disease, chronic rheumatoid arthritis, AIDS, cancer and the like, and having excellent characteristics such as higher avidity, higher biological activity, higher biological stability, higher thermomechanical stability, and higher absorbency to a living body. According to the method of the present invention for designing, identifying, evaluating or searching an effector of the dipeptidyl peptidase IV, there is exhibited an excellent effect that the method can logically and conveniently provide an effector useful as a modulatory agent of immune response and as a therapeutic or prophylactic agent for diabetes, inflammation, multiple sclerosis, Graves' disease, chronic rheumatoid arthritis, AIDS, cancer and the like, and having excellent characteristics such as higher avidity, higher biological activity, higher biological stability, higher thermomechanical stability,

and higher absorbency to a living body. According to the effector of the dipeptidyl peptidase IV of the present invention, there are exhibited excellent effects that the effector is capable of modifying immune response and capable of treating or preventing diabetes, inflammation, multiple sclerosis, Graves' disease, chronic rheumatoid arthritis, AIDS, cancer and the like. Furthermore, according to the program and medium therefor of the present invention, there is exhibited an excellent effect that the method for designing, identifying, evaluating or searching an effector of the dipeptidyl peptidase IV can be performed more rapidly and conveniently.

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The present invention will be hereinafter more specifically explained by the following Examples, but the present invention is not intended to be limited by the Examples in any way. Unless otherwise indicated, the reaction conditions, procedures and the like can be referred to the instruction manual attached to the reagents used, *Molecular Cloning A Laboratory Manual*, third edition, Sambrook et al. [issued by Cold Spring Harbor Laboratory Press (2001)], and the like.

Example 1 Construction of Recombinant Baculovirus for Expression of Soluble Human Dipeptidyl Peptidase IV

20 (1) Cloning of Soluble Human Dipeptidyl Peptidase IV (shDPPIV) cDNA

Caco-2 cells [provided by American Type Culture Collection (ATCC)]

were cultured at 37°C using Dulbecco's Modified Eagle Medium (manufactured by Invitrogen) containing 20% by volume of inactivated fetal bovine serum (manufactured by Invitrogen; inactivated by incubation at 56°C for 30 minutes)

and 1% by volume of nonessential amino acid (manufactured by Invitrogen), in

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the presence of 5% by volume of CO₂.

Next, total RNA was extracted from the Caco-2 cells obtained.

Extraction of the total RNA was carried out using a product manufactured by Nippon Gene Co. Ltd. under the trade name of ISOGEN in accordance with the attached instruction manual. The obtained total RNA was used as a template for RT-nested PCR method described below.

In order to obtain a nucleic acid corresponding to a soluble human DPPIV from which the signal peptide sequence was removed (amino acid nos: 33-766 of SWISS-PROT Accession No: P27487), first, a cDNA fragment sequence of human DPPIV gene was amplified by RT-nested PCR method with total RNA of the Caco-2 as a template.

The thermal profile in the PCR is 30 cycles of reaction, in which one cycle comprises denaturation at 94°C for 30 seconds, annealing at 55°C for 30 seconds and polymerase extension reaction at 72°C for 1 minute.

The amplified DNA fragment was separated by agarose gel electrophoresis method, and a small fragment of the gel of the corresponding band portions was cut out. Thereafter, the DNA fragment was extracted from the obtained small fragments of the gel using a product manufactured by Bio 101 under the trade name of GENE CLEAN SPIN Kit, and purified. The obtained fragment was inserted into vector pCR2.1-TOPO contained in TOPO TA Cloning (registered trade mark) Kit manufactured by Invitrogen to construct pCR-shDPPIV.

In order to confirm whether or not the obtained cDNA fragment encodes the desired polypeptide, deletion mutants regarding the DNA fragment having various lengths were prepared, and a nucleotide sequence for the DNA fragment

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was determined as follows.

First, a DNA fragment having a size of 2.2 kbp obtained by double digestion of the pCR-shDPPIV with BamHI and EcoRI was inserted into a corresponding restriction site in pUC19 (manufactured by Takara Bio Inc.), to construct a plasmid pUshDPPIV. Various deletion plasmids were prepared using the plasmid pUshDPPIV by a conventional method.

The nucleotide sequence for the DNA fragment was determined using the obtained deletion plasmid or plasmid pCR-shDPPIV, and a product manufactured by Perkin-Elmer Cetus Inc. under the trade name of Taq DyeDeoxy Terminator Cycle Sequencing Kit and Model 373S sequencer manufactured by Applied Biosystems.

Also, the amino acid sequence of the polypeptide encoded by the abovementioned DNA fragment was determined on the basis of the nucleotide sequence.

The determined amino acid sequence was compared with the sequence for a full length DPPIV of human colon shown in SEQ ID NO: 2. As a result, it was confirmed that the corresponding regions (regions excluding the transmembrane region) were identical.

Thus, it was confirmed that the DNA fragment encodes the desired polypeptide shDPPIV, namely a polypeptide in which the transmembrane region (amino acid nos: 1-32 at N-terminal side) in the full-length human DPPIV was deleted and a polyhistidine peptide was added to the C-terminal side.

(2) Preparation of Recombinant Baculovirus

Plasmid pUshDPPIV was digested with a restriction enzyme to give a

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DNA fragment encoding shDPPIV gene. The obtained fragment was inserted into pAcGP67B (manufactured by BD PharMingen) to construct a baculovirus transfer vector pAcGP67B-shDPPIV.

Fifteen minutes before the transfection, Sf21 cells were washed twice with a TNM-FH medium comprising 10% by volume of fetal bovine serum. The Sf21 cells were then transferred to a well of a 6-well plate by 2.4×10^6 cells per well.

Furthermore, 2 to 5 µg of the baculovirus transfer vector and a 0.5 µg linear baculovirus DNA (trade name: BaculoGold virus DNA, manufactured by BD PharMingen) were mixed, and the mixture was allowed to stand at room temperature for 5 minutes. Next, 1 ml of Transfection Buffer B (manufactured by BD PharMingen) was added to the obtained mixture, and the mixture was thoroughly mixed to give a Transfection Buffer B/DNA mixture.

The medium in the wells of the 6-well plate and the cells that had not been adhered to the wells were removed, and 1 ml of Transfection Buffer A (manufactured by BD PharMingen) was added to each of the wells. The Transfection Buffer B/DNA mixture was gradually added dropwise to the wells of the 6-well plate, with gently stirring the 6-well plate. The cells were incubated at 28°C for 4 hours in the wells of the 6-well plate. Thereafter, the transfection buffer was removed, and 3 ml of TNM-FH medium containing 10% by volume of fetal bovine serum was added to the wells of the 6-well plate. The cells were cultured at 28°C in each of the wells of the 6-well plate for 5 days, and the culture supernatant was collected. The culture supernatant was used for amplification of virus using Sf21 cells to give a virus stock solution.

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Example 2 Preparation and Crystallization of shDPPIV

(1) Expression of shDPPIV in Insect Cells

(manufactured by JRH Biosciences) and T flask, and Tn5 cells (provided by Invitrogen) were cultured using a serum free medium EX-CELL 401 (manufactured by JRH Biosciences) and a T flask, at 28°C, respectively. At the time when the proliferation of the cells reached 70% confluent, the old medium was removed, and a fresh medium was added at 40 ml per one 225-cm² flask. Then, 1.5 ml of virus stock solution after amplification for three times (having multiplicity of infection (MOI) of about 2) was added to the cells to infect the cells, and the cells were incubated at 28°C for 4 days. The culture supernatant four days after the infection was collected and stored at -20°C. The culture supernatant was used for the purification of shDPPIV protein as described below.

15 (2) Purification of shDPPIV Protein

In each step for the purification of shDPPIV, the activity of DPPIV was measured by incubating a 0.1 ml reaction mixture containing a 1.5 mM substrate [manufactured by Peptide Institute, Gly-Pro-paranitroanilide (pNA)], 71 mM Gly-NaOH (pH 8.7) and the DPPIV, and detecting the liberated pNA.

Meanwhile, the reaction mixture was incubated at 37°C for 10 minutes. During the incubation, the absorbance at 405 nm was monitored.

Also, the protein concentration was quantified by using a product manufactured by Bio-Rad Laboratories, Inc. under the trade name of DC protein Assay Kit II.

The purity of the protein was confirmed by subjecting a protein sample

in each step to SDS-PAGE using 7.5% polyacrylamide gel according to the method by Laemmli et al.

The culture supernatant stored at -20°C in the above-mentioned (1) was melted at 4°C and filtered with a bottle top filter (manufactured by Becton, Dickinson and Company) or with 0.45 µm filter (KURABO INDUSTRIES LTD.) to remove insoluble materials. The supernatant after the filtration was concentrated to an about tenth volume by using a concentrator Vivaflow 50 (manufactured by Sartorius AG) or Amicon stirrer cell model 8400 (manufactured by Millipore Corporation) to give a concentrated solution.

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The obtained concentrated solution was dialyzed against buffer A (20 mM HEPES-NaOH, 0.5 M NaCl, pH 8.0) at 4°C overnight, and applied to a nickel column [one in which nickel was immobilized to HiTrap Chelating column (trade name, manufactured by Amersham-Pharmacia) (5 ml × 2)] equilibrated with buffer A. The column was washed with 10 column volumes of buffer A, and then with buffer A containing 50 mM imidazole. The elution of the fraction containing shDPPIV was carried out by a linear gradient of 50 to 500 mM imidazole. The fraction found to have DPPIV activity was collected, and dialyzed overnight at 4°C against buffer B (20 mM HEPES-NaOH, pH 8.0, 50 mM NaCl). After the dialysis, the sample was purified by using an anion exchange column [manufactured by Amersham-Pharmacia under the trade name: Resource Q (6 ml)] equilibrated with buffer B. The column was washed with buffer B, and thereafter shDPPIV was eluted by a linear gradient of 15 column volumes of 50 to 500 mM NaCl. The fractions found to have DPPIV activity were collected, and used as a purified preparation.

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(3) Preparation of Protein Sample for Crystallization

The shDPPIV purification sample (9 ml) obtained in the above (2) was concentrated using a product manufactured by Millipore Corporation under the trade name of Centricon 10 until the protein concentration reached 10 mg/ml.

The obtained product was used as a protein sample for crystallization.

The protein sample for crystallization was stored at 4°C.

A precipitation agent solution containing 0.18 M glycine-NaOH (pH 9.5), 0.18 M sodium sulfate and 18% by weight of PEG4000, and a 10 mg/ml dipeptidyl peptidase IV solution were mixed, and thereafter, a drop of the obtained mixed solution was placed on a product under the trade name of Cryschem Plate (manufactured by Hampton Research). The above-mentioned precipitation solution was allowed to stand at 20°C as a reservoir solution to allow crystallization.

15 (4) Crystallization of shDPPIV

The crystallization of shDPPIV was carried out by a sitting-drop method, which is one of vapor diffusion methods.

The formation of crystal was observed with the passage of time using a stereoscopic microscope. As a result, after about two weeks, a large crystal having a maximum size of 500 μ m \times 300 μ m \times 100 μ m was obtained. The crystal is also referred to as a native crystal. The microphotograph of the obtained crystal is shown in Figure 1. In Figure 1, the visual field is 4000 μ m \times 3000 μ m.

Example 3 Three-Dimensional Structural Analysis of Crystals

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(1) X-ray Diffraction

The crystal obtained in Example 2 mentioned above was soaked in a cryoprotecting buffer [composition: 0.18 M glycine-NaOH (pH 9.5), 19% by weight of PEG4000, 0.18 M sodium acetate, 15% glycerol], and immediately thereafter the mixture was placed under nitrogen gas stream (100 K) to rapidly freeze the mixture.

The X-ray diffraction intensity data of the above crystal were collected up to the resolution of 3.0Å using a product manufactured by Rigaku International Corporation under the trade name of R-AXIS IV in nitrogen gas stream (100 K), and converted to the structure factor using a program MOSFLM (Version 6.11). A photograph of the diffraction pattern is shown in Figure 2.

From the obtained diffraction intensity data, it was determined that the crystal form to which the crystal belongs was orthorhombic, that the space group was $P2_12_12_1$, and the lattice constants were $a = 118.0 \pm 5.0$ Å, $|b| = 125.9 \pm 5.0$ Å and $|c| = 136.8 \pm 5.0$ Å.

(2) Multiple Isomorphous Replacement Method

In order to derive an electron density map, multiple isomorphous replacement method was carried out. The crystal obtained in Example 2 was soaked for 3 days and 4 days in a crystallization solution prepared by dissolving mercury chloride until being saturated, to give two different kinds of isomorphous replacement crystals containing mercury atoms in the crystals. The X-ray diffraction intensity data were collected in the same manner as those for the native crystals.

In the determination of the phase in the structural analysis, CCP4

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(Collaborative Computational Project, Number 4, 1994. "The CCP4 Suite: Programs for Protein Crystallography," *Acta Cryst.* D50, 760-763) program was used.

First, Fourier transform calculation utilizing the difference between the diffraction intensity obtained from the two kinds of isomorphous replacement crystals of mercury and the diffraction intensity obtained from the native crystal was performed using MLPHERE contained in the CCP program package. The position of each mercury atom in the unit cell of the real space was determined by investigating large peaks provided by heavy atoms (mercury) in the obtained Patterson's diagram. The phase of the crystal structure factor of the native crystals was determined by using the obtained position coordinate of mercury atoms. Furthermore, in order to determine the coordinate of each mercury atom more accurately using DM and SOLOMON contained in the CCP program package, refinement was carried out using three crystal structure factors of the native crystals and of the two kinds of mercury isomorphous replacement crystals.

An electron density map of the crystals of the dipeptidyl peptidase IV in real space was obtained using the phase of the crystal structure factor of the native crystals calculated from the refined coordinates of the mercury atoms. Furthermore, the electron density map was improved by carrying out smoothening and histogram matching of the electron density map in a solvent region, to obtain an electron density map critical for molecular modeling.

(3) Molecular Modeling

The sites corresponding to the amino acid residues of the dipeptidyl

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peptidase IV were identified on the electron density map by using QUANTA (manufactured by Accelrys, Inc.), to build molecular models.

As expected from the lattice constants, there were two molecules of the dipeptidyl peptidase IV in an asymmetry unit, and a model was built for each of the molecules. The refinement of the obtained molecular model was carried out using CNX (manufactured by Accelrys, Inc.), and the molecular model was adjusted again using the QUANTA for the obtained improved electron density map. The procedures were repeated to build a more accurate molecular model. In the refinement of the final coordinate, diffraction intensity data measured again were used after OSMIC confocal mirror (manufactured by Rigaku International Corporation) had been introduced into R-AXIS IV (trade name, manufactured by Rigaku International Corporation).

As a result, the resolution was improved from the previous 3.0Å to 2.6Å. Furthermore, 273 molecules of bound water and 5 molecules of N-acetyl glucosamine residues per molecule of the dipeptidyl peptidase IV were identified in an asymmetric unit. R factor, which is an index for accuracy of the obtained molecular model, was 24.89%, and a free R factor, which independently was not taken into account of the calculation of refinement at the step of refinement, was 30.15%. During the procedure, the deviation of the interatomic bond distance (rms-deviation) and the bond angle from the ideal state of the three-dimensional structure were 0.006Å and 1.305°, respectively. The stereogram of the three-dimensional structure model of the crystals is shown in Figure 3, and the coordinate is shown in Figure 4. The present coordinate data were registered in PDB (Brookhaven Protein Data Bank) [PDB Code No: 1J2E, RSCB code No: 005544].

Here, as to those regions which did not take a regular structure in the crystals (in the disordered state), namely, the region from Asp 38 to that closer to the N-terminal side thereof, and the region for the tagged peptide (polyhistidine peptide) of the C-terminal side, the molecular model could not be built.

Furthermore, a part of the side chains projected to the surface of the molecules did not take a regular structure. However, these residues were not portions that play an important role for the function of enzymes.

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In the three-dimensional structure of the dipeptidyl peptidase IV, which has been clarified by the Examples, it has been revealed that the amino acid residue involved in the activity deduced by various experiments for the dipeptidyl peptidase IV, namely, Ser 630, Asp 708 and His 740, form hydrogen bonds between the $O_{\delta 2}$ atom of Asp 708 and $N_{\delta 1}$ atom of His 740, and with the $N_{\epsilon 2}$ atom of His 740 and O_{γ} atom of Ser 630, even the residues locate in distant locations on the primary sequence. Therefore, for the structural coordinate of Figure 4 and the three-dimensional structure model defined by the structural coordinate, it is suggested that the regions characterized by Ser 630, Asp 708 and His 740, and the whole or a part of amino acid residues that are located in the vicinity of Ser 630, Asp 708 and His 740 play an important role on the exhibition of the activity for the dipeptidyl peptidase IV and binding or interaction of the dipeptidyl peptidase IV with the effector, and that the compound matching the three-dimensional structure of the regions affect the activity for the dipeptidyl peptidase IV.

The present invention may be embodied in other various forms without departing from the spirit or essential characteristics thereof. The present

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embodiment is therefore to be considered in all respects as illustrative and not restrictive, the scope of the invention being indicated by the appended claims rather than by the foregoing description and all changes which come within the meaning and range of equivalency of the claims are therefore intended to be embraced therein.

INDUSTRIAL APPLICABILITY

According to the crystal of the dipeptidyl peptidase IV of the present invention, the information of a three-dimensional structure coordinate suitable for designing, identifying, evaluating or searching an effector of the dipeptidyl peptidase IV, useful as a modulatory agent of immune response and as a therapeutic or prophylactic agent for diabetes, inflammation, multiple sclerosis, Graves' disease, chronic rheumatoid arthritis, AIDS, cancer and the like can be obtained. Also, according to the three-dimensional structure coordinate, the information of a three-dimensional structure coordinate suitable for designing, identifying, evaluating or searching an effector of the dipeptidyl peptidase IV, useful as a modulatory agent of immune response and as a therapeutic or prophylactic agent for diabetes, inflammation, multiple sclerosis, Graves' disease, chronic rheumatoid arthritis, AIDS, cancer and the like can be obtained. Further, according to the method of the present invention for obtaining a threedimensional structure coordinate of a homolog protein of a dipeptidyl peptidase IV, the refinement of the three-dimensional structure coordinate of the homolog protein of the dipeptidyl peptidase IV can be more conveniently carried out. Moreover, according to the method of the present invention for obtaining a threedimensional structure coordinate of a crystal of a complex of a dipeptidyl

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peptidase IV with an effector of the dipeptidyl peptidase IV, the information of a three-dimensional structure coordinate suitable for designing, identifying, evaluating or searching an effector of the dipeptidyl peptidase IV, which is useful as a modulatory agent of immune response and as a therapeutic or prophylactic agent for diabetes, inflammation, multiple sclerosis, Graves' disease, chronic rheumatoid arthritis, AIDS, cancer and the like, and is excellent in avidity, biological activity, biological stability, absorbency to a living body, and which can favorably act on the dipeptidyl peptidase IV can be obtained. Also, according to the method for identifying a pharmacophore of a dipeptidyl peptidase IV and an effector of the dipeptidyl peptidase, the information of a three-dimensional structure coordinate suitable for designing, identifying, evaluating or searching an effector of the dipeptidyl peptidase IV, which is useful as a modulatory agent of immune response and as a therapeutic or prophylactic agent for diabetes, inflammation, multiple sclerosis, Graves' disease, chronic rheumatoid arthritis, AIDS, cancer and the like, and is excellent in avidity, biological activity, biological stability, absorbency to a living body, and which can favorably act on the dipeptidyl peptidase IV can be obtained. Further, according to the method of the present invention for designing, identifying, evaluating or searching an effector of the dipeptidyl peptidase IV, the information of a three-dimensional structure coordinate suitable for designing, identifying, evaluating or searching an effector of the dipeptidyl peptidase IV, which is useful as a modulatory agent of immune response and as a therapeutic or prophylactic agent for diabetes, inflammation, multiple sclerosis, Graves' disease, chronic rheumatoid arthritis, AIDS, cancer and the like, and is excellent in avidity, biological activity, biological stability, absorbency to a living body,

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and which can favorably act on the dipeptidyl peptidase IV can be logically and conveniently obtained. In addition, the effector of the dipeptidyl peptidase IV of the present invention is useful as a modulatory agent of immune response and as a therapeutic or prophylactic agent for diabetes, inflammation, multiple sclerosis, Graves' disease, chronic rheumatoid arthritis, AIDS, cancer and the like. Further, according to the program or the medium therefor of the present invention, the design, identification, evaluation and search for an effector of a dipeptidyl peptidase IV can be carried out rapidly and conveniently. Therefore, the present invention can be utilized in modulation of immune response and the treatment or prevention for diabetes, inflammation, multiple sclerosis, Graves' disease, chronic rheumatoid arthritis, AIDS, cancer and the like.

CLAIMS

- 1. A crystal of a dipeptidyl peptidase IV, having characteristics sufficient to ensure a resolution capable of analyzing its three-dimensional structure up to the side chain level by X-ray crystallographic structural analysis.
- 2. The crystal according to claim 1, wherein the dipeptidyl peptidase IV is a soluble polypeptide comprising a region located at extramembrane in a full-length human dipeptidyl peptidase IV.

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3. The crystal according to claim 1 or 2, wherein the dipeptidyl peptidase IV is a polypeptide having an amino acid sequence in which a transmembrane region is deleted from the amino acid sequence of SEQ ID NO: 2, and a tag peptide is optionally added to a C-terminal side or N-terminal side thereof.

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4. The crystal according to any one of claims 1 to 3, wherein the crystal has a space group of $P2_12_12_1$, and a lattice constant of the unit cell of $|a| = 118.0 \pm 5.0$ Å, $|b| = 125.9 \pm 5.0$ Å, $|c| = 136.8 \pm 5.0$ Å, and $\alpha = \beta = \gamma = 90^{\circ}$, and is orthorhombic.

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- 5. The crystal according to any one of claims 1 to 4, wherein the crystal has the structural coordinate shown in Figure 4.
- 6. The crystal according to any one of claims 1 to 4, wherein the crystal has
 25 a structural coordinate different from the structural coordinate as shown in

Figure 4 via fluctuation of a protein.

- 7. A three-dimensional structural coordinate of a dipeptidyl peptidase IV, comprising the structural coordinate shown in Figure 4.
- 8. A three-dimensional structural coordinate of a dipeptidyl peptidase IV, comprising a structural coordinate different from the structural coordinate as shown in Figure 4 via fluctuation of a protein.
- 9. The three-dimensional structural coordinate according to claim 8, wherein the fluctuation of a protein is a state that is caused by molecular oscillation or temperature, and exhibits an activity for the dipeptidyl peptidase IV in a living body.
- 10. The three-dimensional structural coordinate according to any one of claims 7 to 9, wherein the dipeptidyl peptidase IV is a soluble polypeptide comprising a region located at extramembrane in a full-length human dipeptidyl peptidase IV.
- 20 11. The three-dimensional structural coordinate according to any one of claims 7 to 10, wherein the dipeptidyl peptidase IV is a polypeptide having an amino acid sequence in which a transmembrane region is deleted from the amino acid sequence of SEQ ID NO: 2, and a tag peptide is optionally added of to a Cterminal side or N-terminal side thereof.

- 12. A three-dimensional structural coordinate of a region in a dipeptidyl peptidase IV, comprising the three-dimensional structural coordinate of the region selected from the group consisting of the following (a) to (d):
- (a) a region characterized by Ser 630, Asp 708 and His 740 in the amino acid sequence of SEQ ID NO: 2, and all or a part of a group of the amino acid residues located in the adjacent area of each of the Ser 630, Asp 708 and His 740 in the structural coordinate shown in Figure 4 or the three-dimensional structure model defined by the structural coordinate;
- (b) a region characterized by Ser 630, Asp 708 and His 740 in the amino acid sequence of SEQ ID NO: 2, and all or a part of a group of the amino acid residues comprising amino acids capable of maintaining physicochemical characteristics physiologically equivalent to each of amino acids in the group of the amino acid residues
 located in the adjacent area of each of Ser 630, Asp 708 and His 740, in the structural coordinate shown in Figure 4 or the three-dimensional structure model defined by the structural coordinate,
- (c) a region characterized by a group of amino acid residues comprising amino acids capable of maintaining physicochemical characteristics

 20 physiologically equivalent to each of Ser 630, Asp 708 and His 740 in the amino acid sequence of SEQ ID NO: 2, and all or a part of a group of the amino acid residues located adjacent area of said group of the amino acid residues in the structural coordinate shown in Figure 4 or the three-dimensional structure model defined by the structural coordinate; and

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(d) a region characterized by a group of amino acid residues comprising amino acids capable of maintaining physicochemical characteristics physiologically equivalent to each of Ser 630, Asp 708 and His 740 in the amino acid sequence of SEQ ID NO: 2, and all or a part of a group of amino acid residues comprising amino acids capable of maintaining physicochemical characteristics physiologically equivalent to each of the amino acids in the group of the amino acid residues located in the adjacent area of said group of the amino acids, in the structural coordinate shown in Figure 4 or the three-dimensional structure model defined by the structural coordinate,

wherein the region in the dipeptidyl peptidase IV is a region involved in binding or interaction between the dipeptidyl peptidase IV and an effector of the dipeptidyl peptidase IV.

- 13. The three-dimensional coordinate according to claim 12, wherein the physicochemical characteristic is selected from the group consisting of features in shape of a three-dimensional structure, hydrophobicity, electric charge and pK.
- 14. A method for obtaining a three-dimensional coordinate of a homolog protein of a dipeptidyl peptidase IV, characterized in refining an electron density map of the homolog protein of the dipeptidyl peptidase IV comprising the amino acid sequence of SEQ ID NO: 2, based on all and/or a part of the three-dimensional coordinate of any one of claims 7 to 13, to give a three-dimensional structural coordinate.

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- 15. A method for obtaining a three-dimensional structural coordinate of a crystal of a complex of a dipeptidyl peptidase IV and an effector of the dipeptidyl peptidase IV characterized in using all and/or a part of the three-dimensional structural coordinate of any one of claims 7 to 13, to give a three-dimensional structural coordinate.
- 16. A method for identifying pharmacophore of an effector of the dipeptidyl peptidase IV, characterized in identifying the pharmacophore based on all and/or a part of the three-dimensional structural coordinate of any one of claims 7 to 13, and the steric conformation of the effector of the dipeptidyl peptidase IV.
- 17. A method for designing, identifying, evaluating or searching an effector of a dipeptidyl peptidase IV, characterized in designing, identifying, evaluating or searching a compound capable of acting on the dipeptidyl peptidase IV, based on all and/or a part of the three-dimensional structural coordinate of any one of claims 7 to 13.
- 18. The method according to claim 17, wherein the method for designing, identifying, evaluating or searching an effector comprises the steps of:
- 20 (i) identifying a region to be targeted for binding or interaction with the effector in a dipeptidyl peptidase IV, based on all and/or a part of the three-dimensional structural coordinate according to any one of claims 7 to 13 and the steric conformation of the effector of the dipeptidyl peptidase IV;
- 25 (ii) identifying atoms or atomic groups capable of generating in the above

region at least one intermolecular interaction selected from the group consisting of covalent bond, ionic interaction, ion-dipole interaction, dipole-dipole interaction, hydrogen bonding, van der Waals force, electrostatic interaction and hydrophobic interaction, with the atoms or atomic groups existing in a candidate compound; and

(iii) designing a compound based on the information of the above step (i) and/or (ii).

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19. The method according to claim 18, wherein the method further comprises the steps of:

detecting an interaction between the dipeptidyl peptidase IV and the designed, identified, evaluated or searched candidate compound, wherein when an interaction is detected, the candidate compound is identified as a compound capable of binding to the dipeptidyl peptidase IV, based on a degree of the interaction as an index.

20. The method according to claim 18 or 19, wherein the method further comprises the steps of:

contacting the dipeptidyl peptidase IV with the designed, identified,
evaluated or searched candidate compound and measuring an activity of the
dipeptidyl peptidase IV,
wherein when an activity increases or decreases, the designed, identified,
evaluated or searched candidate compound is identified as a compound having
enhancing action or inhibitory action on the activity of the dipeptidyl peptidase
IV, based on a degree of the increase or decrease as an index.

- 21. An effector of the dipeptidyl peptidase IV obtainable by the method of any one of claims 17 to 20.
- 5 22. A program and a medium therefor for use of the three-dimensional structural coordinate of any one of claims 7 to 13, wherein all and/or a part of the three-dimensional structural coordinate of any one of claims 7 to 13 is recorded.
- 23. The program and the medium according to claim 22, comprising a means for identifying, searching, evaluating or designing a compound capable of binding to the dipeptidyl peptidase IV or a compound having an enhancing action or inhibitory action on the activity for the dipeptidyl peptidase IV.
- 24. The program and the medium according to claim 23, further comprising a means for displaying a three-dimensional graphic display of a molecule.

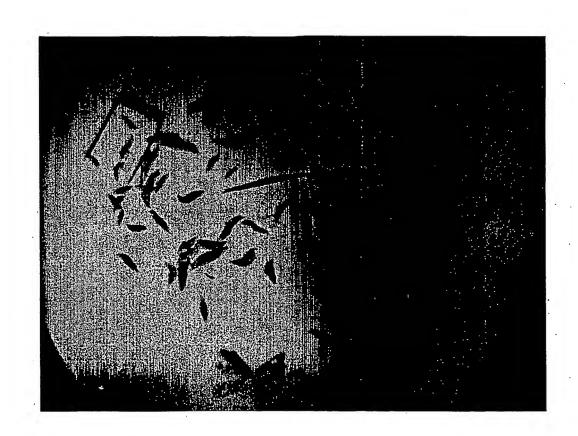
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FIG. 1



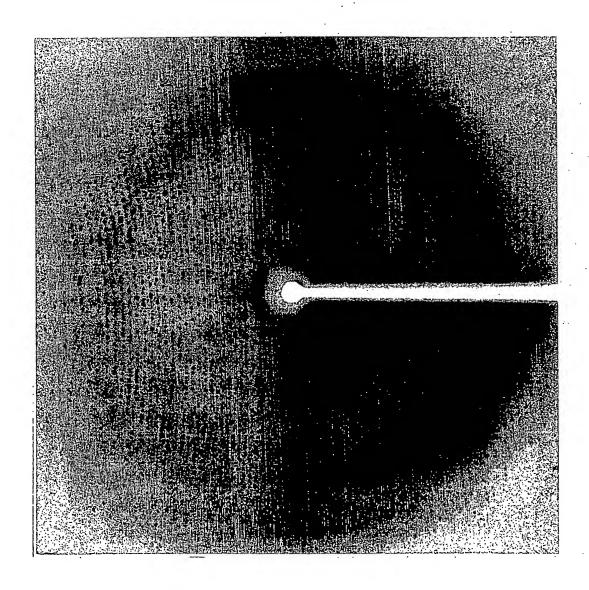
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FIG. 2



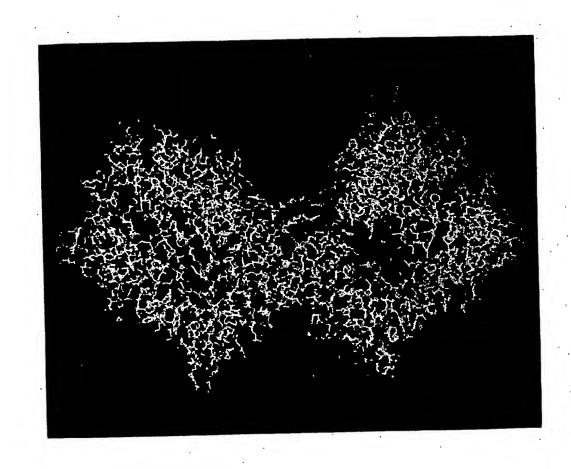
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FIG. 3



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F I G. 4 - 1

	T	hree-	-dime	nsional	structural	coordin	ate of	dipeptidyl	peptidase	IV
ATOM	1	СВ	ASP	38	44. 493	31.885	58. 92	7 1.00 42.	46 A	С
ATOM	2	CG	ASP	38	44. 146	32.095	57.46			Č
ATOM	3	0D1	ASP	38	43.664	33. 198	57.13			0
ATOM	4	0D2		38	44.360	31.171	56.65			0
ATOM	5	C	ASP	38	45.876	29.805	58.63			Č
ATOM	6	Ö	ASP	38	46.980	30.327	58.77			0
ATOM	7	N	ASP	38	44. 758	30.264	60.77			N
ATOM	8	CA	ASP	38	44.639	30.404	59.29			C
ATOM	9	N	SER	39	45.679	28.711	57.90	5 1.00 40.	69 A	N
ATOM	10	CA	SER	39	46. 775	28.013	57. 24			C
ATOM	11	CB	SER	39	46. 584	26.501	57.38		43 A	C
ATOM	12	0G	SER	39	45.410	26.079	56.70			0
ATOM	13	C	SER	39	46. 960	28.343	55.76			C
ATOM	14	0	SER	39	47.870	27.813	55.12			0
ATOM	15	N	ARG	40	46.093	29. 190	55.21			N
ATOM	16	CA	ARG	40	46. 194	29.575	53.81			C
ATOM	17	CB	ARG	40	45.082	30.558	53.43			C
ATOM	18	CG	ARG	40	43.683	29.984	53.40			C
ATOM	19	CD	ARG	40	42.688	31.098	53. 13			C
ATOM	20	NE	ARG	40	42.774	32.134	54.16			N
MOTA	21	CZ	ARG	40	42.097	33. 276	54.12			C
ATOM	22	NH1	ARG	40	41. 280	33. 528	53.11			N
ATOM	23		ARG	40	42. 239	34. 167	55.09		_ :	N
ATOM ATOM	24 25	C 0	ARG ARG	40	47. 530	30. 251	53. 53			C
ATOM	26	N	LYS	40 41	48. 100 48. 031	30. 901 30. 100	54. 40 52. 31			0
ATOM	27	CA	LYS	41	49. 286	30. 749	51.93			N
ATOM	28	CB	LYS	41	49. 705	30. 338	50. 52		•	C
ATOM	29	CG	LYS	41	48. 684	30. 719	49.46			C
ATOM	30	CD	LYS	41	49. 026	30. 151	48. 09			Č
ATOM	31	CE	LYS	41	47. 805	30. 201	47.17			Č
ATOM	32	NZ	LYS	41	48. 070	29. 686	45. 79			Ň
ATOM	33	C	LYS	41	49. 038	32. 257	51.95			Ċ
ATOM	34	Ö	LYS	41	47. 891	32. 715	51.98			ő
ATOM	35	N	THR	42	50.110	33. 032	51.95			Ň
ATOM	36	CA	THR	42	49. 967	34. 479	51.93			C
ATOM	37	CB	THR	42	50.860	35. 139	53.00			Č
ATOM	38		THR	42	52. 234	34.843	52.72			0
ATOM	39	CG2	THR	42	50. 501	34.622	54.38			C
ATOM	40	C	THR	42	50. 389	34. 971	50.55			C
ATOM	41	0	THR	42	50. 977	34. 220	49.78			0
ATOM	42	N	TYR	43	50. 058	36. 217	50. 23			N
ATOM	43	CA	TYR	43	50.465	36. 782	48. 95			С
ATOM	44	CB	TYR	43	49.615	38.006	48. 623			C
ATOM	45	CG	TYR	43	49.922	38. 625	47. 28			C
ATOM	46	CD1	TYR	43	50.977	39.527	47. 130			C
ATOM	47	CE1	TYR	43	51. 253	40.113	45. 89		_	C
ATOM	48	UDZ	TYR	43	49. 152	38. 315	46. 158	3 1.00 26.4	10 A	C

				(Continued)
			FIG. 4-2	
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	49 CE2 TYR 50 CZ TYR 51 OH TYR 52 C TYR 53 O TYR 54 N THR 55 CA THR 56 CB THR 57 OG1 THR 60 O THR 61 N LEU 62 CA LEU 63 CB LEU 63 CB LEU 64 CG LEU 65 CD1 LEU 66 CD2 LEU 67 C LEU 68 O LEU 67 C LEU 68 O LEU 67 C THR 72 OG1 THR 72 OG1 THR 72 OG1 THR 72 OG1 THR 73 CG2 THR 74 C THR 75 O THR 75 O THR 76 N ASP 77 CA ASP 78 CB ASP 80 OD1 ASP 81 OD2 ASP 80 OD1 ASP 81 OD2 ASP 82 C ASP 83 O ASP 84 N TYR 85 CA TYR 86 CB TYR 87 CG TYR 88 CD1 TYR	43 43 43 44 44 44 44 44	49. 424 38. 891 44. 919 1. 00 25. 89 50. 473 39. 790 44. 796 1. 00 25. 91 50. 741 40. 370 43. 579 1. 00 25. 09 51. 933 37. 165 49. 160 1. 00 24. 97 52. 251 38. 049 49. 955 1. 00 23. 33 52. 818 36. 482 48. 444 1. 00 24. 06 54. 255 36. 685 48. 580 1. 00 25. 90 54. 960 35. 336 48. 547 1. 00 25. 86 54. 960 34. 709 47. 285 1. 00 28. 12 54. 439 34. 436 49. 655 1. 00 22. 61 54. 917 37. 576 47. 530 1. 00 27. 35 54. 918 37. 956 46. 535 1. 00 27. 39 56. 978 38. 722 46. 853 1. 00 26. 43 58. 377 38. 954 47. 425 1. 00 26. 07 59. 310 39. 860 46. 612 1. 00 26. 21 58. 734 41. 263 46.	(Continued) A C C C A C C C A C C C A C C C A C C C A C C C A C C C A C C C A C C C A C C C A C
ATOM ATOM ATOM	88 CD1 TYR 89 CE1 TYR 90 CD2 TYR	48 48 48	53. 460 42. 971 42. 609 1. 00 23. 19 53. 703 44. 184 41. 982 1. 00 24. 84 55. 694 42. 946 43. 461 1. 00 25. 89	A C
ATOM ATOM	91 CE2 TYR 92 CZ TYR	48 48	55. 956 44. 165 42. 838 1. 00 26. 76 54. 955 44. 779 42. 096 1. 00 27. 28	A C A C A O
ATOM ATOM ATOM	93 OH TYR 94 C TYR 95 O TYR	48 48 48	54. 820 39. 953 41. 796 1. 00 28. 80 54. 445 40. 401 40. 714 1. 00 28. 24	A C A 0
ATOM ATOM	96 N LEU 97 CA LEU	49 49	56.054 39.499 41.988 1.00 29.41 57.046 39.552 40.918 1.00 30.39	A N A C

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					17. 1		0			(Continued)
					F I	G. 4	- 3			
ATOM	98	СВ	LEU	49	58. 455	39.318	41.481	1.00 27.73	Α	C
ATOM	99	CG	LEU	49	58. 988	40.473	42. 336	1.00 28.28	A	C
ATOM	100		LEU	49	60. 438	40. 223	42.711	1.00 26.99	A	C
ATOM	101		LEU	49	58.860	41. 773 38. 606	41.555 39.752	1.00 26.02 1.00 30.71	A A	C
ATOM ATOM	102 103	C 0	LEU LEU	49 49	56.804 57.147	38. 919	38. 614	1.00 30.11	A	ŏ
ATOM	103	N	LYS	50	56. 198	37. 459	40. 024	1.00 32.51	Ä	Ň
ATOM	105	CA	LYS	50	55.959	36. 491	38. 971	1.00 33.54	A	Ċ
ATOM	106	CB	LYS	50	56.289	35.098	39.485	1.00 33.30	Α	С
ATOM	107	CG	LYS	50	57. 763	34.940	39. 790	1.00 33.89	A .	С
ATOM	108	CD	LYS	50	58. 591	35. 213	38. 545	1.00 35.19	A	C
ATOM	109	CE	LYS	50	60.071	34. 945	38. 778	1.00 38.12	A	C
ATOM	110	NZ	LYS	50	60.859	35.028	37. 515	1.00 39.27	A	N
ATOM ATOM	111	C	LYS LYS	50 50	54. 572 54. 272	36. 517 35. 719	38. 361 37. 478	1.00 34.93 1.00 35.13	A A	C 0
ATOM	112 113	O N	ASN	50 51	53. 731	37. 436	38. 822	1.00 36.66	A	N
ATOM	114	CA	ASN	51	52. 379	37. 569	38. 294	1.00 38.39	A	Ċ
ATOM	115	CB	ASN	51	52. 428	37. 859	36. 791	1.00 41.61	A	Č
ATOM	116	CG	ASN	51	53.407	38.968	36.436	1.00 44.75	Α	C
ATOM	117		ASN	51	53. 212	40.131	36.801	1.00 46.38	Α	0
ATOM	118		ASN	51	54.470	38. 609	35. 717	1.00 45.80	A	N
ATOM	119	C	ASN	51	51.529	36. 324	38. 517	1.00 38.21	A	C
ATOM	120	0	ASN	51	50.708	35.976	37.674	1.00 40.60	A	0
ATOM ATOM	121 122	N CA	THR THR	52 52	51.720 50.942	35. 647 34. 451	39. 641 39. 926	1.00 36.74 1.00 35.44	A A	N C
ATOM	123	CB	THR	52 52	51.297	33. 888	41. 298	1.00 35.44	A	Č
ATOM	124	0G1		52 52	52.646	33.415	41. 272	1.00 38.62	A	ŏ
ATOM	125		THR	52	50. 367	32. 750	41.666	1.00 35.25	A	Č
ATOM	126	C	THR	52	49.431	34.686	39.869	1.00 35.17	Α	Ċ
ATOM	127	0	THR	52	48.699	33.889	39. 276	1.00 36.44	Α	0
ATOM	128	N	TYR	53	48.962	35. 765	40. 487	1.00 33.55	Α	N
ATOM	129	CA	TYR	53	47. 535	36.081	40. 487	1.00 33.46	A	C
ATOM	130	CB	TYR	53	47.084	36. 407	41.903	1.00 32.64	A	C
ATOM ATOM	131 132	CG CD1	TYR TYR	53 53	47. 399 48. 341	35. 293 35. 462	42. 861 43. 872	1.00 33.83 1.00 34.11	A A	C C
ATOM	133	CE1	TYR	53	48. 657	34. 425	44.741	1.00 34.11	A	Č
ATOM	134		TYR	53	46. 775	34.050	42. 741	1.00 36.17	A	č·
ATOM	135	CE2		53	47.084	33.001	43.605	1.00 35.64	Ä	č
ATOM	136	CZ	TYR	53	48.026	33.199	44.601	1.00 35.74	A	Č
ATOM	137	OH	TYR	53	48. 343	32.170	45.453	1.00 35.79	Α	0
ATOM	138	Č.	TYR	53	47. 266	37. 248	39. 548	1.00 33.40	A	С
ATOM	139	0	TYR	53	47. 486	38. 404	39. 895	1.00 33.56	A	0
ATOM	140	N	ARG	54 54	46.773	36. 929	38. 355	1.00 34.36	A	N
ATOM .	141 142	CA CB	ARG ARG	54 54	46. 526 46. 993	37. 933	37. 327	1.00 34.87	A	C C
ATOM ATOM	142	CG	ARG	54 54	46. 887	37. 387 38. 373	35. 972 34. 821	1.00 35.72 1.00 39.96	A A	C
ATOM	144	CD	ARG	54 54	47. 675	37. 880	33. 613	1.00 33.30	A	Č
ATOM	145	NE	ARG	54	47.651	38. 831	32. 506	1.00 46.70	A	Ň
ATOM	146	CZ	ARG	54	46.587	39.068	31.744	1.00 49.10	A	С

	• •			(Continued)
			FIG. 4-4	
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	147 NH1 ARG 148 NH2 ARG 149 C ARG 150 O ARG 151 N LEU 152 CA LEU 153 CB LEU 154 CG LEU 155 CD1 LEU 156 CD2 LEU 157 C LEU 158 O LEU 159 N LYS 160 CA LYS 161 CB LYS 162 CG LYS 163 CD LYS 164 CE LYS 165 NZ LYS 166 C LYS 167 O LYS 168 N LEU 170 CB LEU 170 CB LEU 170 CB LEU 171 CG LEU 171 CG LEU 171 CG LEU 172 CD1 LEU 173 CD2 LEU 174 C LEU 175 O LEU 176 N TYR 177 CA TYR 178 CB TYR 179 CG TYR 178 CB TYR 179 CG TYR 180 CD1 TYR 181 CE1 TYR 182 CD2 TYR 183 CE2 TYR 184 CZ TYR 185 OH TYR 187 O TYR 188 N SER 189 CA SER 190 CB SER 191 OG SER 191 OG SER 191 OG SER 192 C SER 193 O SER 194 N LEU 195 CA LEU	5444455555555555555555555555555555555	## F I G. 4 - 4 45. 451	A A A A A A A A A A A A A A A A A A A
ATOM	195 CA LEU	•	CURATITUTE CHEET (DUI E 26)	

				(Continued)
			FIG. 4-5	
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	196 CB LEU 197 CG LEU 198 CD1 LEU 199 CD2 LEU 200 C LEU 201 O LEU 201 O LEU 202 N ARG 203 CA ARG 204 CB ARG 205 CG ARG 206 CD ARG 207 NE ARG 208 CZ ARG 209 NH1 ARG 211 C ARG 211 C ARG 211 C ARG 212 O ARG 213 N TRP 214 CA TRP 215 CB TRP 216 CG TRP 217 CD2 TRP 218 CE2 TRP 219 CE3 TRP 210 CD1 TRP 211 NE1 TRP 222 CZ2 TRP 223 CZ3 TRP 224 CH2 TRP 225 C TRP 226 O TRP 227 N ILE 228 CA ILE	60 60 60 60 60 61 61 61 61 61 61 62 62 62 62 62 62 62 62 62 62 62 63 63	FIG. 4 - 5 36. 256	A C C C C C C C C C C C C C C C C C C C
ATOM ATOM ATOM ATOM	229 CB ILE 230 CG2 ILE 231 CG1 ILE 232 CD1 ILE	63 63 63	35. 312 48. 727 14. 180 1. 00 25. 95 36. 494 48. 000 14. 783 1. 00 27. 39 34. 092 47. 810 14. 138 1. 00 24. 70 34. 246 46. 666 13. 174 1. 00 25. 35	A C A C A C A C A C
ATOM ATOM ATOM ATOM ATOM	233 C ILE 234 O ILE 235 N SER 236 CA SER 237 CB SER	63 63 64 64	33. 788 50. 680 14. 400 1. 00 26. 00 33. 803 51. 075 13. 239 1. 00 26. 14 32. 738 50. 812 15. 202 1. 00 26. 48 31. 510 51. 470 14. 768 1. 00 28. 43 30. 764 50. 603 13. 754 1. 00 27. 24	A 0 A N A C A C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM	238 OG SER 239 C SER 240 O SER 241 N ASP 242 CA ASP 243 CB ASP 244 CG ASP	64 64 64 65 65 65	30. 181 49. 481 14. 392 1. 00 28. 00 30. 597 51. 727 15. 964 1. 00 29. 08 31. 008 51. 606 17. 119 1. 00 26. 71 29. 348 52. 067 15. 678 1. 00 31. 29 28. 382 52. 336 16. 732 1. 00 34. 90 27. 384 53. 397 16. 269 1. 00 37. 81 26. 515 53. 905 17. 395 1. 00 41. 52	A

	•					
				FIG. 4-6		(Continued)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	246 247 248 249 250 251 252 253 254 255 256 257	OD1 ASP OD2 ASP C ASP O ASP O ASP O HIS CA HIS CB HIS CCB HIS	65566666666666666666666666666666666666	FIG. 4 - 6 27. 070	AAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAA	OOCONCCCNCNCONCCCCOOCONCCCCCCCCONCCCCCONCCCCCC

				FIG. 4-7		(Continued)
ATOM	294	CD2 TYR	70	37. 421 39. 563 23. 213 1. 00 43. 93	A	С
ATOM	295	CE2 TYR	70	37. 853 39. 104 24. 452 1. 00 44. 83	A	C
ATOM	296	CZ TYR	70	00.000	A	C
ATOM	297	OH TYR	70	00.001	A	0
ATOM	298	C TYR	70	00.210	A	C
ATOM	299	O TYR	70	00.010 00.102 2.102	A	0 N
ATOM	300	N LYS	71	40. 254 40. 231 21. 072 1. 00 49. 93	A	N
ATOM	301	CA LYS	71	41.113 39.064 20.895 1.00 54.71	A	C C
ATOM	302	CB LYS	71	42. 580 39. 460 21. 054 1. 00 54. 14	A	C
ATOM	303	CG LYS	71	43. 075 40. 455 20. 031 1. 00 56. 37	A	C
ATOM	304	CD LYS	71	44.559 40.712 20.226 1.00 58.61 45.126 41.628 19.159 1.00 58.78	A A	C
ATOM	305	CE LYS	71		A	N N
ATOM	306	NZ LYS	71		A	Č
ATOM	307	C LYS	71	40. 790 37. 952 21. 889 1. 00 57. 38 41. 109 38. 062 23. 075 1. 00 58. 38	A	ŏ
ATOM	308	O LYS	$\begin{array}{c} 71 \\ 72 \end{array}$	40. 158 36. 884 21. 406 1. 00 60. 30	A	Ň
ATOM	309	N GLN CA GLN	72	39. 816 35. 750 22. 261 1. 00 63. 23	Ä	Ċ
ATOM ATOM	310 311	CA GLN CB GLN	72	38. 902 34. 775 21. 526 1. 00 64. 07	Ä	Č
ATOM	312	CG GLN	72	38. 313 33. 695 22. 417 1. 00 65. 84	Ā	Č
ATOM	313	CD GLN	72	37. 270 34. 240 23. 375 1. 00 66. 33	A	С
ATOM	314	OE1 GLN	72	36. 251 34. 790 22. 952 1. 00 67. 19	A	0
ATOM	315	NE2 GLN	72	37. 519 34. 092 24. 671 1. 00 66. 80	A	N
ATOM	316	C GLN	72	41.122 35.049 22.607 1.00 65.34	A	С
ATOM	317	O GLN	72	41.563 35.058 23.760 1.00 67.00	A	0
ATOM	318	N GLU	73	41.736 34.442 21.597 1.00 66.09	A	N
ATOM	319	CA GLU	73	43.012 33.763 21.775 1.00 67.12	A	C
ATOM	320	CB GLU	73	43.008 32.420 21.046 1.00 68.53	A	C
ATOM	321	CG GLU	73	41.974 31.433 21.570 1.00 71.35	A	C
ATOM	322	CD GLU	73	42. 223 31. 026 23. 012 1. 00 72. 71	A	C
ATOM	323	OE1 GLU	73	41. 491 30. 147 23. 517 1. 00 73. 51	A	0
ATOM	324	OE2 GLU	73	43. 147 31. 585 23. 643 1. 00 74. 16	A	0
ATOM	325	C GLU	73	44.076 34.681 21.184 1.00 66.83	A	C
ATOM	326	O GLU	73	44. 563 35. 592 21. 857 1. 00 67. 65	A	0 N
ATOM	327	N ASN	74	44. 430 34. 442 19. 924 1. 00 65. 38 45. 411 35. 273 19. 236 1. 00 63. 38	A A	C
ATOM	328	CA ASN	74		A	C
ATOM	329	CB ASN	74		A	č
ATOM	330	CG ASN	74	47. 654 34. 422 20. 034 1. 00 66. 10 48. 128 35. 463 20. 496 1. 00 65. 51	A	ŏ
ATOM	331 332	OD1 ASN ND2 ASN	74 74	47. 973 33. 216 20. 503 1. 00 66. 62	Ä	Ň
ATOM	333	C ASN	74	44. 794 35. 859 17. 977 1. 00 61. 55	Ä	Ċ
ATOM ATOM	334	O ASN	74	45. 384 36. 714 17. 318 1. 00 62. 15	A	Ö
ATOM	335	N ASN	75	43.597 35.390 17.647 1.00 58.67	Ä	N
ATOM	336	CA ASN	75	42.888 35.886 16.481 1.00 55.82	A	Ĉ.
ATOM	337	CB ASN	75	42. 023 34. 785 15. 871 1. 00 57. 81	A	Ċ
ATOM	338	CG ASN	75	41. 410 33. 887 16. 916 1. 00 58. 63	Α	С
ATOM	339	OD1 ASN	75	40.857 34.358 17.909 1.00 59.69	Α	0
ATOM	340	ND2 ASN	75	41, 500 32, 580 16, 697 1, 00 58, 92	A	N
ATOM	341	C ASN	7 5	42.017 37.045 16.918 1.00 52.82	A	C
ATOM	342		75	41.630 37.135 18.081 1.00 53.60	A	0

					FΙ	G. 4	- 9			(Continued)
ATOM	392	CB (GLU	82	22.602	44. 794	19.655	1.00 36.97	Α	С
ATOM	393		GLU	82	21.115	44.827	19.968	1.00 40.49	Α	C
ATOM	394		GLU	82	20.313	45.538	18.894	1.00 44.05	A	C
ATOM	395	0E1		82	20.343	45.087	17.726	1.00 45.13	A	0
ATOM	396	0E2		82	19.652	46.551	19. 220	1.00 45.61	A	0
ATOM	397		GLU	82	23.042	42.853	21. 153	1.00 33.95	A	C
ATOM	398		GLU	82	22.055	42.662	21.864	1.00 32.29	A	0
ATOM	399	N '	TYR	83	23.777	41.857	20.666	1.00 33.23	A	N C
ATOM	400		TYR	83	23. 423	40.468	20.947	1.00 33.39	A	C
ATOM	401		TYR	83	22. 846	39.810	19.686	1.00 34.54	A A	C
ATOM	402		TYR	83	21.690	40.594	19.109	1.00 34.80 1.00 35.22	A	Č
ATOM	403		TYR	83	20.558	40.859	19. 878 19. 396	1.00 35.22	A	Č
ATOM	404	CE1		83	19.527	41.657 41.139	17.828	1.00 35.71	Ä	č
ATOM	405	CD2		83	21.759 20.731	41.139	17. 331	1.00 37.42	Ä	č
ATOM	406	CE2		83 83	19. 619	42.200	18. 125	1.00 37.70	A	Č
ATOM	407		TYR TYR	83	18. 624	43.044	17.675	1.00 37.69	Ā	0
ATOM ATOM	408 409		TYR	83	24. 582	39.644	21. 494	1.00 33.19	Ā	С
ATOM	410		TYR	83	24. 396	38. 511	21.934	1.00 32.91	Α	0
ATOM	411		GLY	84	25. 777	40.217	21.476	1.00 33.53	A	N
ATOM	412		GLY	84	26.933	39.513	21.995	1.00 33.40	Α	C
ATOM	413		GLY	84	27. 454	38.395	21.114	1.00 33.92	A	C
ATOM	414		GLY	84	28. 329	37.639	21.530	1.00 33.21	A	0
ATOM	415	N	ASN	85	26.918	38. 269	19.904	1.00 35.26	A	N
ATOM	416	CA	ASN	85	27. 388	37. 233	18.993	1.00 37.43	A	C
ATOM	417	CB	ASN	85	26. 258	36.780	18.072	1.00 38.34	A	C C
ATOM	418	CG	ASN	85	25. 764	37.878	17.166	1.00 40.02	A A	0
ATOM	419	OD1		85	25. 694	39.040	17. 561 15. 950	1.00 39.96 1.00 41.91	A	N
ATOM	420	ND2		85	25. 394	37. 496 37. 794	18. 188	1.00 38.80	A	Č
ATOM	421	C	ASN	85 85	28. 556 28. 687	39.011	18. 035	1.00 40.05	A	ŏ
ATOM	422	0	ASN SER	85 86	29. 410	36. 920	17.670	1.00 39.14	Ä	Ň
ATOM	423 424	N CA	SER	86	30. 565	37. 393	16. 926	1.00 39.30	Ä	Ċ
ATOM ATOM	425	CB	SER	86.	31. 723	37. 587	17.895	1.00 38.90	A	С
ATOM	426	OG	SER	86	32. 041	36.356	18.515	1.00 35.77	A	0
ATOM	427	C	SER	86	31.023	36.482	15.798	1.00 39.94	A	С
ATOM	428		SER	86	30. 287	35.622	15.323	1.00 41.15	A	0
ATOM	429	N	SER	87	32. 264	36.701	15.382	1.00 40.59	A	N
ATOM	430	CA	SER	87	32.916	35. 929	14.333	1.00 40.98	A	C
ATOM	431	CB	SER	87	32. 152	36.053	13.010	1.00 39.16	A	C
ATOM	432	0G	SER	87	31.727	37. 376	12. 789	1.00 39.90	A	0
ATOM	433		SER	87	34. 353	36. 433	14. 194		A	C
ATOM	434		SER	87	34. 691	37. 517	14.682	1.00 41.07	A A	O N
ATOM	435		VAL	88	35. 206	35.646	13.548		A	
ATOM	436		VAL	88	36. 596	36.043	13. 402 13. 114		A	C C
ATOM	437		VAL	88	37. 502	34. 836 35. 295	13.114		A	Č
ATOM	438		VAL	88	38. 949 37. 361	35. 295 33. 808	14. 222		A	Č
ATOM	439		VAL	88 88	36. 827	33. 606 37. 096	12. 331	1.00 41.63	Ä	č
ATOM	440	С	VAL	00	JU. 041	01.000	12.001			

٠	•	(Continued	I)
	FIG. 4-10		
ATOM 441 0 VAL ATOM 442 N PHE ATOM 443 CA PHE ATOM 444 CB PHE ATOM 445 CG PHE ATOM 446 CD1 PHE ATOM 447 CD2 PHE ATOM 449 CE2 PHE ATOM 450 CZ PHE ATOM 451 C PHE ATOM 451 C PHE ATOM 452 O PHE ATOM 453 N LEU ATOM 454 CA LEU ATOM 455 CB LEU ATOM 456 CG LEU ATOM 457 CD1 LEU ATOM 458 CD2 LEU ATOM 459 C LEU ATOM 459 C LEU ATOM 460 O LEU ATOM 461 N GLU ATOM 461 N GLU ATOM 462 CA GLU ATOM 463 CB GLU ATOM 464 CG GLU ATOM 465 CD GLU ATOM 465 CD GLU ATOM 466 OE1 GLU ATOM 467 OE2 GLU ATOM 468 C GLU ATOM 469 O GLU ATOM 470 N ASN ATOM 471 CA ASN ATOM 473 CG ASN ATOM 474 OD1 ASN ATOM 474 OD1 ASN ATOM 475 ND2 ASN	89 37. 343 38. 238 12. 767 1. 00 89 37. 641 39. 347 11. 880 1. 00 89 37. 769 40. 637 12. 699 1. 00 89 37. 990 41. 865 11. 870 1. 00 89 39. 217 42. 103 11. 265 1. 00 89 36. 963 42. 778 11. 678 1. 00 89 39. 415 43. 231 10. 480 1. 00 89 37. 154 43. 911 10. 894 1. 00 89 38. 381 44. 135 10. 295 1. 00 89 38. 956 39. 021 11. 186 1. 00 89 39. 156 39. 335 10. 019 1. 00 90 41. 143 38. 001 11. 380 1. 00 90 42. 071 39. 213 11. 366 1. 00 90 43. 033 39. 305 10. 184 1. 00 90 42. 236 39. 408 8. 889 1. 00 90 42. 063 37. 159 13. 421 1. 00	(Continued 41. 38	D
ATOM 465 CD GLU ATOM 466 OE1 GLU ATOM 467 OE2 GLU ATOM 468 C GLU ATOM 469 O GLU ATOM 470 N ASN ATOM 471 CA ASN	91 41. 875 30. 694 10. 350 1. 0 91 40. 566 31. 833 9. 001 1. 0 91 43. 855 34. 521 12. 588 1. 0 91 44. 572 34. 841 11. 641 1. 0 92 44. 322 34. 117 13. 766 1. 0 92 45. 738 34. 028 14. 100 1. 0 92 45. 881 33. 389 15. 477 1. 0	0 63.50 A 0 0 63.04 A 0 0 56.96 A C 0 56.93 A 0 0 57.64 A N 0 58.91 A C	
ATOM 474 OD1 ASN ATOM 475 ND2 ASN ATOM 476 C ASN ATOM 477 O ASN ATOM 478 N SER ATOM 479 CA SER ATOM 480 CB SER ATOM 481 OG SER ATOM 482 C SER ATOM 483 O SER ATOM 484 N THR	92 45.189 31.248 14.684 1.0 92 44.420 31.894 16.691 1.0 92 46.622 33.271 13.111 1.0 92 47.806 33.061 13.370 1.0 93 46.059 32.862 11.984 1.0 93 46.828 32.127 10.991 1.0 93 45.978 30.985 10.427 1.0 93 46.714 30.198 9.507 1.0 93 47.296 33.030 9.853 1.0 93 48.314 32.765 9.213 1.0 94 46.552 34.103 9.618 1.0	00 59.97 A O	
ATOM 485 CA THR ATOM 486 CB THR ATOM 487 OG1 THR ATOM 488 CG2 THR ATOM 489 C THR	94 45. 982 36. 298 8. 659 1. 0 94 46. 469 37. 302 7. 759 1. 0 94 46. 003 36. 821 10. 080 1. 0	00 63. 25 A C 00 63. 59 A O 00 64. 14 A C 00 62. 28 A C	

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				(Continued)
			FIG. 4-11	
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	490 O THR 491 N PHE 492 CA PHE 493 CB PHE 494 CG PHE 495 CD1 PHE 496 CD2 PHE 497 CE1 PHE 498 CE2 PHE 500 C PHE 501 O PHE 502 N ASP 503 CA ASP 504 CB ASP 505 CG ASP 506 OD1 ASP 507 OD2 ASP 508 C ASP 508 C ASP 509 O ASP 510 N GLU 511 CA GLU 512 CB GLU	94 95 95 95 95 95 95 96 96 96 96 97 97 97	48. 882 35. 295 7. 303 1. 00 61. 92 A 48. 908 36. 013 9. 426 1. 00 62. 57 A 50. 290 36. 473 9. 322 1. 00 63. 04 A 50. 414 37. 889 9. 897 1. 00 61. 98 A 49. 456 38. 869 9. 289 1. 00 61. 01 A 48. 248 39. 155 9. 911 1. 00 60. 97 A 49. 742 39. 473 8. 073 1. 00 60. 73 A 47. 337 40. 026 9. 330 1. 00 60. 46 A 48. 838 40. 343 7. 483 1. 00 60. 09 A 47. 633 40. 621 8. 113 1. 00 61. 07 A 51. 346 35. 571 9. 956 1. 00 63. 20 A 52. 178 36. 035 10. 736 1. 00 63. 20 A 52. 178 36. 035 10. 736 1. 00 63. 37 A 51. 323 34. 288 9. 611 1. 00 63. 37 A 52. 298 33. 347 10. 149 1. 00 64. 05 A 51. 771 31. 913 10. 044 1. 00 65. 11 A 50. 747 31. 589 11. 115 1. 00 65. 73 A 49. 758 32. 342 11. 240 1. 00 66. 41 A 50. 929 30. 580 11. 829 1. 00 65. 32 A 53. 621 33. 470 9. 399 1. 00 63. 82 A 54. 696 33. 433 10. 001 1. 00 64. 05 A 53. 540 33. 619 8. 083 1. 00 62. 95 A 54. 740 33. 754 7. 271 1. 00 62. 73 A 54. 596 32. 964 5. 965 1. 00 65. 91	
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	513 CG GLU 514 CD GLU 515 OE1 GLU 516 OE2 GLU 517 C GLU 518 O GLU 519 N PHE 520 CA PHE 521 CB PHE 522 CG PHE 523 CD1 PHE 524 CD2 PHE 525 CE1 PHE 526 CE2 PHE 527 CZ PHE 527 CZ PHE 528 C PHE 529 O PHE 529 O PHE 530 N GLY 531 CA GLY 531 CA GLY 532 C GLY 533 O GLY 534 N HIS 535 CA HIS 536 CB HIS 537 CG HIS 537 CG HIS 538 CD2 HIS	97 97 97 97 97 97 98 98 98 98 98 98 98 99 99 100 100 100	54. 954 31. 478 6. 064 1. 00 68. 84 A 53. 945 30. 657 6. 850 1. 00 70. 64 A 54. 160 29. 432 6. 988 1. 00 71. 38 A 52. 939 31. 228 7. 325 1. 00 71. 80 A 55. 039 35. 220 6. 963 1. 00 60. 82 A 55. 462 35. 557 5. 857 1. 00 60. 31 A 54. 818 36. 084 7. 952 1. 00 58. 68 A 55. 067 37. 513 7. 797 1. 00 55. 93 A 54. 200 38. 319 8. 765 1. 00 55. 47 A 54. 272 39. 801 8. 542 1. 00 54. 84 A 53. 712 40. 372 7. 404 1. 00 53. 89 A 55. 032 41. 997 9. 226 1. 00 53. 18 A 55. 032 41. 997 9. 226 1. 00 52. 22 A 56. 536 37. 820 8. 060 1. 00 54. 61	C C C C C C C C C C C C C C C C C C C

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CA

SER

ATOM

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(Continued) FIG. 4-12 ٠, 60.170 41.627 10.346 1.00 49.70 N ND1 HIS 100 ATOM 539 41.951 9.259 1.00 49.10 A C CE1 HIS 60.848 **ATOM** 540 100 N 60.015 41.949 8.234 1.00 50.14 A 100 ATOM 541 NE2 HIS C 57.011 39.511 12.810 1.00 48.06 A HIS 100 542 C **ATOM** 55.920 38.977 12.602 1.00 47.18 A 0 HIS 543 0 100 **ATOM** 57.377 39.958 14.005 1.00 46.66 A N SER 101 **ATOM** 544 N C 39.878 15.136 - 1.00 45.88 A 56.467 SER 101 **ATOM** 545 CA C 39.802 16.446 1.00 47.41 A 57.247 101 CB SER **ATOM** 546 58.118 38.685 16.447 1.00 51.04 A 0 **ATOM** 547 0G SER 101 C 41.142 15.112 1.00 44.53 A 55.617 SER 101 548 C **ATOM** 42.248 0 56.133 15.282 1.00 44.41 A 0 SER 101 549 **ATOM** N 54.319 40.976 14.877 1.00 41.90 A ILE 102 N **ATOM** 550 53.409 42.109 14.833 1.00 38.95 C A 102 ATOM CA ILE 551 C 41.732 14.117 1.00 38.54 52.106 A 102 **ATOM** 552 CB ILE Č 1.00 38.18 51.153 42.926 14.103 A CG2 ILE **ATOM** 553 102 41.288 12.686 1.00 37.65 52.424 A **ATOM** 554 CG1 ILE 102 C 40.733 11.937 1.00 37.11 A CD1 ILE 102 51.243 **ATOM** 555 C 16.244 1.00 38.00 42.597 556 C ILE 102 53.104 A **ATOM** 0 41.919 17.024 1.00 38.06 557 0 ILE 102 52.441 A **ATOM** 53.601 43.787 16.556 1.00 37.54 A N ASN 103 **ATOM** 558 N 53.429 44.399 17.867 C 1.00 36.65 A ASN 103 **ATOM** 559 CA 1.00 37.69 C 54.437 45.530 18.039 A CB ASN 103 560 **ATOM** 54.219 46.308 19.315 1.00 39.56 C Α ASN 103 561 CG **ATOM** 54.655 45.891 20.388 1.00 43.00 0 A OD1 ASN 103 **ATOM** 562 19.211 1.00 38.34 N 53.528 47.439 A ND2 ASN 103 **ATOM** 563 C 52.031 44.953 18.116 1.00 35.79 A ASN 564 C 103 **ATOM** 51.532 44.910 19.237 1.00 35.79 A 0 ASN ATOM 565 0 103 51.405 45.490 17.078 N 1.00 34.43 A **ATOM** 566 N ASP 104 C 50.079 46.067 17.236 1.00 33.27 A CA ASP 104 ATOM 567 C 50.200 47.388 17.998 1.00 34.38 ASP A **ATOM** CB 104 568 C 48.896 47.823 18,618 1.00 34.79 A ASP 569 CG 104 ATOM 0 48.699 19.509 1.00 33.92 A ATOM OD1 ASP 48.916 104 570 18.207 47.289 1.00 36.80 0 OD2 ASP 47.852 A 571 104 **ATOM** 49.436 46.281 15.865 1.00 32.32 C **ASP** A 572 C 104 **ATOM** 50.124 46.326 14.850 1.00 32.03 0 A ASP 104 **ATOM** 573 0 1.00 31.15 15.834 48.118 46.405 N 574 N TYR 105 Α **ATOM** 47.421 46.580 14.570 1.00 32.24 C CA 105 Α **ATOM** 575 TYR 46.672 45.296 14.223 1.00 34.70 A C 105 **ATOM** 576 CB TYR C 45.443 45.088 15.072 1.00 37.73 Α **TYR** 105 ATOM 577 CG C 44.220 45.636 14.698 1.00 37.51 A 578 CD1 TYR 105 **ATOM** 43.098 45.510 15.506 1.00 40.43 A C TYR ATOM 579 CE1 105 45.514 44.395 16.284 C 1.00 39.06 A **ATOM** 580 CD2 TYR 105 44.263 17.103 1,00 40.75 C 44.393 CE2 TYR A **ATOM** 581 105 16.705 C 44.829 1.00 41.19 43.191 Α 582 CZ TYR 105 ATOM 44.755 17.519 1.00 44.27 A 0 42.088 **ATOM** 583 0H TYR 105 1.00 31.43 C A 47.743 14.638 **ATOM** 584 C TYR 105 46.441 1.00 30.78 0 48.249 15.715 A 585 TYR 105 46.133 ATOM 0 1.00 30.16 13.479 N 48.152 586 106 45.940 Α ATOM N SER

SUBSTITUTE SHEET (RULE 26)

45.000

49.261

13.415

1.00 29.23

C

A

			EIC 4-13	(Continued)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	588 CB SER 589 OG SER 590 C SER 591 O SER 591 O SER 592 N ILE 593 CA ILE 594 CB ILE 595 CG2 ILE 596 CG1 ILE 597 CD1 ILE 598 C ILE 597 CD1 ILE 598 C ILE 599 O ILE 600 N SER 601 CA SER 602 CB SER 603 OG SER 604 C SER 605 O SER 606 N PRO 607 CD PRO 608 CA PRO 609 CB PRO 600 CG PRO 610 CG PRO 611 C PRO 612 O PRO 612 O PRO 613 N ASP 614 CA ASP 615 CB ASP 616 CG ASP 617 OD1 ASP 618 OD2 ASP 619 C ASP 617 OD1 ASP 618 OD2 ASP 619 C ASP 610 CG ASP 617 OD1 ASP 618 OD2 ASP 619 C ASP 617 OD1 ASP 618 OD2 ASP 619 C ASP 617 OD1 ASP 618 OD2 ASP 619 C ASP 617 OD1 ASP 618 OD2 ASP 619 C ASP 617 OD1 ASP 618 OD2 ASP 619 C ASP 617 OD1 ASP 618 OD2 ASP 610 CG ASP 617 OD1 ASP 618 OD2 ASP 619 C ASP 610 CG ASP 617 OD1 ASP 618 OD2 ASP 619 C ASP 610 CG ASP 611 C BLN 632 C GLN 633 C GLN 634 N PHE 635 CA PHE	106 106 106 107 107 107 107 107 107 107 107 107 108 108 108 109 109 109 109 110 110 110 110 111 111	## F I G. 4 - 1 3 ## 4.924 51.668 13.090 1.00 32.32 44.146 49.187 12.157 1.00 27.65 44.657 49.085 11.051 1.00 28.57 42.835 49.240 12.331 1.00 28.07 41.922 49.171 11.198 1.00 27.70 40.648 48.352 11.544 1.00 25.83 39.557 48.620 10.522 1.00 26.35 40.970 46.859 11.551 1.00 25.36 41.980 46.457 12.568 1.00 23.77 41.502 50.556 10.743 1.00 26.85 41.178 51.420 11.557 1.00 26.55 41.507 50.757 9.432 1.00 26.55 41.507 50.757 9.432 1.00 26.30 40.458 51.119 6.700 1.00 23.63 39.639 52.253 9.169 1.00 27.22 38.857 51.310 9.206 1.00 26.49 39.241 53.506 9.393 1.00 27.22 38.857 51.310 9.206 1.00 26.49 39.241 53.506 9.393 1.00 28.50 40.025 54.751 9.302 1.00 29.19 37.839 53.794 9.693 1.00 29.19 37.845 55.294 9.439 1.00 28.76 36.842 52.993 8.852 1.00 29.21 35.901 52.425 9.391 1.00 28.76 36.842 52.993 8.852 1.00 29.21 35.901 52.425 9.391 1.00 28.76 36.842 52.993 8.852 1.00 29.21 35.901 52.425 9.391 1.00 28.76 36.842 52.993 8.852 1.00 29.21 36.120 52.202 6.676 1.00 28.98 36.241 52.673 5.226 1.00 27.99 37.613 52.425 9.391 1.00 29.41 36.120 52.202 6.676 1.00 28.98 36.241 52.673 5.226 1.00 27.99 37.613 52.425 9.391 1.00 29.41 36.280 50.685 6.715 1.00 29.53 37.349 48.766 7.702 1.00 28.14 37.890 48.064 6.470 1.00 29.53 37.856 46.837 6.402 1.00 29.53 37.856 46.837 6.402 1.00 31.76 48.818 5.503 1.00 29.53 37.856 46.837 6.402 1.00 31.16 38.405 48.818 5.503 1.00 29.53 37.856 46.837 6.402 1.00 31.79 37.191 50.234 1.465 1.00 30.99 43 40.415 47.813 4.981 1.00 30.627 38.314 50.644 48.818 5.503 1.00 29.74 38.77 49.171 3.109 1.00 29.74 38.77 49.171 3.109 1.00 29.74 38.77 49.171 3.109 1.00 29.74 38.77 49.171 3.109 1.00 29.94 37.336 49.442 2.749 1.00 31.79 37.191 50.234 1.465 1.00 31.79 37.191 50.234 1.465 1.00 31.79 37.191 50.234 1.465 1.00 31.79 37.191 50.234 1.465 1.00 31.79 37.191 50.234 1.465 1.00 31.79 37.191 50.234 1.465 1.00 31.79 37.191 50.234 1.465 1.00 32.82 343.428 49.207 4.900 1.00 24.48	A C O C C C C C C O N C C C C O N C C C C

	FIG. 4-14	(Continued)
ATOM 637 CG PHE 113 ATOM 638 CD1 PHE 113 ATOM 639 CD2 PHE 113 ATOM 640 CE1 PHE 113 ATOM 641 CE2 PHE 113 ATOM 642 CZ PHE 113 ATOM 642 CZ PHE 113 ATOM 643 C PHE 113 ATOM 644 O PHE 113 ATOM 645 N ILE 114 ATOM 646 CA ILE 114 ATOM 646 CA ILE 114 ATOM 647 CB ILE 114 ATOM 649 CG1 ILE 114 ATOM 650 CD1 ILE 114 ATOM 651 C ILE 114 ATOM 652 O ILE 114 ATOM 653 N LEU 115 ATOM 654 CA LEU 115 ATOM 655 CB LEU 115 ATOM 656 CG LEU 115 ATOM 656 CG LEU 115 ATOM 657 CD1 LEU 115 ATOM 658 CD2 LEU 115 ATOM 660 O LEU 115 ATOM 661 N LEU 116 ATOM 662 CA LEU 116 ATOM 663 CB LEU 116 ATOM 664 CG LEU 116 ATOM 665 CD1 LEU 116 ATOM 667 C LEU 116 ATOM 667 C LEU 116 ATOM 668 O LEU 116 ATOM 667 C LEU 116 ATOM 667 C LEU 116 ATOM 668 O LEU 116 ATOM 667 C LEU 116 ATOM 667 C LEU 116 ATOM 668 O LEU 116 ATOM 667 C LEU 117 ATOM 671 CB GLU 117 ATOM 672 CG GLU 117 ATOM 673 CD GLU 117 ATOM 673 CD GLU 117 ATOM 674 OEI GLU 117 ATOM 673 CD GLU 117	## 1 G. 4 - 1 4 43. 193	A A A A A A A A A A A A A A A A A A A
ATOM 674 OE1 GLU 117 ATOM 675 OE2 GLU 117 ATOM 676 C GLU 117 ATOM 677 O GLU 117	52. 732 49. 572 17. 268 1.00 29. 08 52. 552 51. 242 15. 868 1.00 30. 62 53. 997 46. 491 13. 738 1.00 27. 81 53. 666 45. 586 14. 506 1.00 27. 41	A 0 A 0 A C A 0
ATOM 678 N TYR 118 ATOM 679 CA TYR 118 ATOM 680 CB TYR 118 ATOM 681 CG TYR 118 ATOM 682 CD1 TYR 118 ATOM 683 CE1 TYR 118 ATOM 684 CD2 TYR 118 ATOM 685 CE2 TYR 118	55. 247 46. 663 13. 313 1. 00 27. 75 56. 327 45. 796 13. 765 1. 00 29. 68 56. 473 44. 586 12. 837 1. 00 29. 52 56. 819 44. 903 11. 402 1. 00 28. 58 55. 922 45. 572 10. 573 1. 00 29. 31 56. 236 45. 838 9. 239 1. 00 28. 13 58. 040 44. 510 10. 864 1. 00 28. 81 58. 362 44. 769 9. 541 1. 00 27. 91	A N A C A C A C A C A C A C A C A C A C

				(Continued)
			FIG. 4-15	
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	686 CZ TYR 687 OH TYR 688 C TYR 689 O TYR 690 N ASN 691 CA ASN 692 CB ASN 693 CG ASN 694 OD1 ASN 695 ND2 ASN 696 C ASN 697 O ASN 698 N TYR 700 CB TYR 700 CB TYR 700 CB TYR 701 CG TYR 702 CD1 TYR 703 CE1 TYR 704 CD2 TYR 705 CE2 TYR 706 CZ TYR 707 OH TYR 708 C TYR 707 OH TYR 708 C TYR 707 OH TYR 708 C TYR 709 O TYR 700 CZ TYR 701 CA VAL 711 CA VAL 712 CB VAL 713 CG1 VAL 714 CG2 VAL 715 C VAL 716 O VAL 717 N LYS 718 CA LYS 719 CB LYS 720 CG LYS		FIG. 4 - 15 57. 459	(Continued) A
ATOM ATOM ATOM	721 CD LYS 722 CE LYS 723 NZ LYS	122	59.078 53.406 27.174 1.00 19.23 60.062 54.510 27.346 1.00 18.20	A C A N
ATOM ATOM ATOM ATOM ATOM ATOM	724 C LYS 725 O LYS 726 N GLN 727 CA GLN 728 CB GLN 729 CG GLN	122 123 123 123	61. 460 53. 635 22. 528 1. 00 27. 64 62. 658 53. 464 22. 315 1. 00 28. 10 60. 947 54. 813 22. 860 1. 00 27. 23 61. 791 55. 979 23. 071 1. 00 27. 82 61. 607 57. 034 21. 974 1. 00 28. 29 62. 537 58. 227 22. 164 1. 00 28. 94	A C A O A N A C A C A C
ATOM ATOM ATOM ATOM ATOM	730 CD GLN 731 OE1 GLN 732 NE2 GLN 733 C GLN 734 O GLN	123 123 123 123	62. 339 59. 308 21. 131 1. 00 29. 91 61. 218 59. 744 20. 889 1. 00 32. 37 63. 431 59. 761 20. 524 1. 00 30. 94 61. 385 56. 545 24. 428 1. 00 26. 89 61. 837 56. 036 25. 453 1. 00 27. 03	A C A O A N A C A O

(Continued)

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									00 00	. А	NI.
ATOM	735	N	TRP	124	60.522	57. 564	24. 444		23.89	Α	N
ATOM	736		TRP	124	60.081	58.149	25. 713		24. 21	Α	C
			TRP	124	59.886	59.665	25. 572	1.00	23.25	Α	С
ATOM	737		TRP	124	61.052	60.357	24. 934	1.00	19.79	Α	С
ATOM	738	CG			62.444	60.061	25. 127		19.03	Α	С
ATOM	739		TRP	124			24. 270		19.13	A	C
ATOM	740		TRP	124	63. 175	60. 913		1.00	15.51	Ä	č
ATOM	741		TRP	124	63. 143	59. 157	25. 936		18.84	A	č
ATOM	742	CD1	TRP	124	60. 999	61.350	24.006				N
ATOM	743	NE 1	TRP	124	62.270	61.690	23.597		18. 74	A	C
ATOM	744	CZ2	TRP	124	64. 571	60.885	24. 196		17.77	A	C
ATOM	745	CZ3	TRP	124	64.533	59.129	25.860		15. 41	A	
ATOM	746	CH2	TRP	124	65.229	59.986	24.996		17.07	A	C
ATOM	747	C	TRP	124	58. 787	57. 494	26. 209		24. 57	A	C
ATOM	748	0	TRP	124	58.490	56. 350	25.861		25. 71	A	0
ATOM	749	Ň	ARG	125	58.013	58. 218	27.013	1.00		A	Ŋ
ATOM	750	CA	ARG	125	56.779	57.670	27.567	1.00		A	C
ATOM	751	CB	ARG	125	56.189	58.621	28.609	1.00	23.81	Α	C
ATOM	752	CG	ARG	125	54.953	58.065	29.308	1.00	23.85	Α	C
ATOM	753	CD	ARG	125	54. 273	59.129	30.143	1.00	26. 24	Α	C
	754	NE	ARG	125	55.090	59.579	31.269	1.00	25.99	Α	N
ATOM		CZ	ARG	125	55. 293	58.867	32. 372		26.04	Α	C
ATOM	755 756		ARG	125	56.051	59. 357	33. 347		24.42	Α	N
ATOM	756	NH1		125	54. 735	57.668	32. 500		25. 19	A	N
ATOM	757	NH2			55. 706	57. 324	26. 541	1.00		A	
ATOM	758	C	ARG	125	54. 935	56. 387	26. 752		25.04	A	
ATOM	759	0	ARG	125			25. 436		23. 33	A	
ATOM	760	N	HIS	126	55.651	58.063	24. 403		22.86	A	
ATOM	761	CA	HIS	126	54. 649	57. 800		1.00		A	
ATOM	762	CB	HIS	126	53.649	58. 943	24. 353		22.35	A	
ATOM	763	CG	HIS	126	52. 987	59. 224	25.662			A	
ATOM	764	CD2		126	53.027	60.316	26.463		21.51		
ATOM	765		HIS	126	52.137	58. 329	26. 274		22.03	A	
ATOM	766		HIS	126	51.679	58. 859	27. 395	1.00		A	
ATOM	767	NE2	HIS	126	52. 202	60.064	27.532	1.00		A	
ATOM	768	C	HIS	126	55. 222	57. 599	22.995	1.00		A	
ATOM	769	0	HIS	126	54. 599	56.947	22. 153		23.99	A	
ATOM	770	N	SER	127	56.40 1	58. 163	22.744	1.00		P	
ATOM	771	CA	SER	127	57.039	58. 072	21.434	1.00		P	
ATOM	772	CB	SER	127	58.050	59. 213	21.267	1.00		P	
ATOM	773	0G	SER	127	58.909	59.311	22. 387	1.00	23.05	P	
ATOM	774		SER	127	57.737	56.748	21.146	1.00	24.40	P	V C
ATOM	775	ŏ	SER	127	58.167	56.050		1.00	26.55	. A	0
ATOM	776		TYR	128	57.841	56.420		1.00	22.67	. A	N N
	777	CA	TYR	128	58. 501	55. 207	19.403		22.06	ŀ	7 . C
ATOM			TYR	128	57. 787	53. 962			21.99	I	/ C
ATOM	778			128	56. 413	53. 712			22.49		À Č
ATOM	779		TYR		55. 257	54. 112			23. 20		i č
ATOM	780					53. 857			19.81		i č
ATOM	781				53.992				20.70		i č
ATOM	782		2 TYR		56. 267	53.049			20. 70		À Č
ATOM	783	CE	2 TYR	128	55.007	52. 791	17. 580	1.00	J 40.01		

		DIC 4-17	(Continued)
		FIG. 4 - 17	A C
ATOM	784 CZ TYR 128	00.012	A 0
ATOM	785 OH TYR 128	08.011	A Č
ATOM	786 C TYR 128	00.000	Å Ö
ATOM	787 0 TYR 128	01.000	A N
ATOM	788 N THR 129		A C
ATOM	789 CA THR 129		A C
ATOM	790 CB THR 129 791 OG1 THR 129		A 0
ATOM			A C
ATOM .	792 CG2 THR 129 793 C THR 129	59, 062 52, 675 15, 580 1, 00 24, 85	A C
ATOM ATOM	794 0 THR 129	59, 168 51, 811 16, 457 1, 00 22, 29	A 0
ATOM	795 N ALA 130	58. 692 52. 411 14. 337 1. 00 24. 54	A N
ATOM	796 CA ALA 130	00.000 01.002 10.010	A C
ATOM	797 CB ALA 130	01.001	A C
ATOM	798 C ALA 130	00.150	A C A 0
ATOM	799 O ALA 130	30.21	A O A N
ATOM	800 N SER 131	01.010	A C
ATOM	801 CA SER 131	0,000,000,000	Ä Č
ATOM	802 CB SER 13	10.000 10.000	A 0
ATOM	803 OG SER 13 804 C SER 13	10 100 1 17	A C
ATOM	804 C SER 13 805 O SER 13	11 00 07 00	A 0
ATOM ATOM	806 N TYR 13	55, 747 49, 351 9, 232 1, 00 27, 56	A N
ATOM	807 CA TYR 13	54. 341 49. 061 9. 029 1. 00 28. 28	A C
ATOM	808 CB TYR 13	53. 532 50. 357 9. 156 1. 00 27. 16	A C
ATOM	809 CG TYR 13	53.649 51.046 10.507 1.00 25.23	A C
ATOM	810 CD1 TYR 13	52. 692 50. 842 11. 500 1. 00 24. 00	A C
ATOM	811 CE1 TYR 13		A C
ATOM	812 CD2 TYR 13		A C
ATOM	813 CE2 TYR 13	1000 00 00	A C
ATOM	814 CZ TYR 13	1 100 1 00 01 00	A Ö
ATOM	815 OH TYR 13 816 C TYR 13		Ä Č
ATOM		0 710 1 00 00 54	A 0
ATOM	817 0 TYR 13 818 N ASP 13	7	A N
ATOM ATOM	819 CA ASP 13	3 52.629 46.956 6.392 1.00 31.05	A C
ATOM	820 CB ASP 13	3 53.147 45.519 6.314 1.00 31.90	A C
ATOM	821 CG ASP 13	3 54, 541 45, 436 5, 721 1, 00 33, 92	A C
ATOM	822 OD1 ASP 13	3 54.773 46.042 4.649 1.00 33.52	A 0
ATOM	823 OD2 ASP 13		A 0
ATOM	824 C ASP 13		A C A O
ATOM	825 0 ASP 13		A O A N
ATOM	826 N ILE 13		A C
ATOM	827 CA ILE 13	1 00 00 01	A Č
ATOM	828 CB ILE 13		Ä Č
ATOM	829 CG2 ILE 13 830 CG1 ILE 13		A C
ATOM	830 CG1 ILE 13 831 CD1 ILE 13	4 49 232 51, 277 3, 846 1, 00 22, 40	A C
ATOM ATOM	832 C ILE 1	1 = 0.4 + 0.0 0.7 A.C.	A C
AIOm	יו ממו ט מטט		

				(Continued)
•			FIG. 4-18	
ATOM	833 0 ILE	134	49.171 45.894 3.521 1.00 27.19 A	0 .
ATOM	834 N TYR	135	47, 599 45, 805 5, 127 1, 00 29, 43 A	
ATOM	835 CA TYR	135	46. 985 44. 588 4. 628 1. 00 30. 54 A	
ATOM	836 CB TYR	135	46. 800 43. 588 5. 772 1. 00 33. 25 A	
ATOM	837 CG TYR	135	46. 276 42. 242 5. 343 1. 00 35. 66 A	
ATOM	838 CD1 TYR	135	47. 113 41. 311 4. 731 1. 00 37. 89 A	
ATOM	839 CE1 TYR	135	46. 634 40. 068 4. 319 1. 00 40. 13 A	C
ATOM	840 CD2 TYR	135	44. 939 41. 903 5. 535 1. 00 37. 34 A	
ATOM	841 CE2 TYR	135	44. 444 40. 666 5. 126 1. 00 40. 17 A 45. 296 39. 751 4. 518 1. 00 41. 67 A	
ATOM	842 CZ TYR	135	10. 200 00. 101	
ATOM	843 OH TYR	135	1 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2	
ATOM.	844 C TYR	135	45. 629 44. 990 4. 057 1. 00 30. 05 A 44. 870 45. 705 4. 704 1. 00 28. 31 A	
ATOM	845 0 TYR 846 N ASP	135 136	45. 341 44. 536 2. 841 1. 00 31. 33 A	
ATOM	846 N ASP 847 CA ASP	136	44. 083 44. 837 2. 168 1. 00 33. 02 A	
ATOM ATOM	848 CB ASP	136	44.323 44.857 0.655 1.00 32.51 A	
ATOM	849 CG ASP	136	43.057 45.095 -0.146 1.00 33.01 A	
ATOM	850 OD1 ASP	136	43.115 45.872 -1.121 1.00 31.21 A	_
ATOM	851 OD2 ASP	136	42.009 44.500 0.181 1.00 34.97 A	_
ATOM	852 C ASP	136	43. 019 43. 797 2. 549 1. 00 35. 55	
ATOM	853 O ASP	136	42. 822 42. 810 1. 846 1. 00 36. 12	
ATOM	854 N LEU	137	42.341 44.040 3.669 1.00 38.03 A	
ATOM	855 CA LEU	137	11.000	
ATOM	856 CB LEU	137	40. 445 43. 892 5. 225 1. 00 40. 10 F 41. 160 44. 413 6. 477 1. 00 39. 13 F	_
ATOM	857 CG LEU 858 CD1 LEU	137 137		Ā Č
ATOM ATOM	858 CD1 LEU 859 CD2 LEU	137		A C
ATOM	860 C LEU	137		A C
ATOM	861 0 LEU	137	40.038 41.362 3.225 1.00 43.41	0 A
ATOM	862 N ASN	138	39. 997 43. 322 2. 141 1. 00 45. 42	A N
ATOM	863 CA ASN	138	00.100	A C
ATOM	864 CB ASN	138	00.001	A C
ATOM	865 CG ASN	138	011111	A C A O
MOTA	866 OD1 ASN	138	00.010	A O A N
ATOM	867 ND2 ASN	138	00.202	A C
ATOM	868 C ASN	138 138		A Ö
ATOM	869 0 ASN 870 N LYS	139		A N
ATOM ATOM	870 N LYS 871 CA LYS	139		A C
ATOM	872 CB LYS	139	42, 510 42, 374 -2, 382 1, 00 51, 15	A C
ATOM	873 CG LYS	139	41.785 43.427 -3.212 1.00 53.38	A C
ATOM	874 CD LYS	139	42.753 44.331 -3.974 1.00 54.25	A C
ATOM	875 CE LYS	139	10.000	A C
ATOM	876 NZ LYS	139	11. 11.	A N
ATOM	877 C LYS	139	10. 110	A C A 0
ATOM	878 0 LYS	139	40.110	A O A N
ATOM	879 N ARG		18.800 1.00 1.00 1.00 1.00	A C
ATOM	880 CA ARG			Ä Č
ATOM	881 CB ARG	140	44.000 00.400 1.010 1.00 00.00	

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					FΙ	G. 4	- 19			(00111111111111111111111111111111111111
		00	400	1.40	40.011	90 405	0 157	1 00 57 96	٨	C
ATOM	882	CG	ARG	140	40.911	38. 495	2. 157	1.00 57.36 1.00 60.02	A A	C
ATOM	883	CD	ARG	140	40. 257 40. 936	37. 128 36. 235	2. 211 3. 142	1.00 60.02	A	N
ATOM	884	NE C7	ARG ARG	140 140	40. 633	34. 950	3. 294	1.00 64.87	A	Č
ATOM	885	CZ NH1	ARG	140	39. 661	34. 409	2. 570	1.00 66.83	A	Ň
ATOM ATOM	886 887		ARG	140	41. 298	34. 206	4. 169	1.00 65.62	A	N
ATOM	888	C	ARG	140	44. 464	39. 603	1.066	1.00 50.29	A	Ċ
ATOM	889	ŏ	ARG	140	44. 992	38. 496	1.002	1.00 50.21	A	0
ATOM	890	N	GLN	141	45. 096	40. 723	0. 741	1.00 49.82	A	N
ATOM	891	CA	GLN	141	46. 473	40.707	0. 268	1.00 48.70	Α	С
ATOM	892	CB	GLN	141	46. 487	40.815	-1.260	1.00 50.32	Α	С
ATOM	893	CG	GLN	141	47. 774	40.348	-1.909	1.00 55.02	Α	С
ATOM	894	CD	GLN	141	47.640	40.179	-3.413	1.00 57.33	Α	С
ATOM	895	0E1	GLN	141	48.582	39.756	-4.088	1.00 57.97	Α	0
ATOM	896	NE2	GLN	141	46.465	40.509	-3.947	1.00 58.85	Α	Ŋ
ATOM	897	С	GLN	141	47. 293	41.837	0.898	1.00 46.02	A	C
ATOM	898	0	GLN	141	46. 761	42.880	1. 274	1.00 45.33	A	0
ATOM	899	N	LEU	142	48. 594	41.610	1.013	1.00 43.34	A	N
ATOM	900	CA	LEU	142	49. 505	42.578	1.605	1.00 41.50	A	C
ATOM	901	CB	LEU	142	50. 638	41.824	2.296	1.00 41.17	A	C
ATOM	902	CG	LEU	142	51.489	42.501	3. 359	1.00 42.33	A	C
ATOM	903		LEU	142	52. 443 52. 254	41.463	3. 922	1.00 42.24	A	C
ATOM	904		LEU	142	02.201	43.677	2.772	1.00 42.66 1.00 40.87	A	C C
ATOM	905	C	LEU LEU	$\begin{array}{c} 142 \\ 142 \end{array}$	50. 062 50. 557	43. 498 43. 030	0. 520 -0. 506	1.00 40.87	A A	0
ATOM ATOM	906 907	O N	ILEU	142	49. 978	44. 806	0.748	1.00 41.31	A	N N
ATOM	908	CA	ILE	143	50.466	45. 789	-0.217	1.00 37.17	A	Č
ATOM	909	CB	ILE	143	49. 921	47. 202	0. 104	1.00 36.58	A	č
ATOM	910		ILE	143		48. 225	-0.874	1.00 35.56	A	č
ATOM	911		ILE	143	48. 398	47. 197	0.030	1.00 34.64	A	č
ATOM	912		ILE	143	47.777	48. 494	0.468	1.00 37.28	A	č
ATOM	913	C	ILE	143	51.985	45.843	-0. 209	1.00 36.06	A	Č.
ATOM	914	Ŏ	ILE	143	52.603	45.859	0.849	1.00 36.63	A	Ő.
ATOM	915	N	THR	144	52. 592	45.882	-1.386	1.00 35.40	Α	N
ATOM	916	CA	THR	144	54.046	45.933	-1.459	1.00 35.79	A	С
ATOM	917	CB	THR	144	54.616	44.654	-2.124	1.00 35.59	Α	С
ATOM	918	.0G1	THR	144	54. 192	44.592	-3.491	1.00 37.13	Α	0
ATOM	919		THR	144	54. 121	43. 415	-1.403	1.00 33.21	A	С
ATOM	920	C	THR	144	54. 515	47. 152	-2. 243	1.00 35.43	A	C
ATOM	921	0	THR	144	55. 700	47.311	-2.511	1.00 36.45	A	0
ATOM	922	N	GLU	145	53. 577	48.015	-2.602	1.00 36.27	A	Ŋ
ATOM	923	CA	GLU	145	53. 891	49. 214	-3. 369	1.00 36.32	A	C
ATOM	924	CB	GLU	145	52.962	49. 297	-4.586	1.00 38.36	A	C
ATOM	925	CG	GLU	145	53. 553	48. 748	-5.875	1.00 42.66	A	C
ATOM	926	CD	GLU	145	54.667	49.639	-6.418	1.00 45.91	A	C
ATOM	927		GLU	145	55. 745	49. 705	-5. 779	1.00 45.49	A	0
ATOM	928		GLU	145	54. 456 52. 775	50. 283	-7. 476 -2. 544	1.00 45.56 1.00 35.06	Α	0 C
ATOM	929	C	GLU	145	53. 775 52. 874	50. 496 50. 635	-2. 544 -1. 715	1.00 35.00	A A	0
ATOM	930	0	GLU	145	J4. 014	au. 0aa	-1.710	1.00 04.66	и	U

		° FIG. 4-	2 0		((Continued)
ATOM 937 0E2 ATOM 938 C ATOM 939 0 ATOM 940 N ATOM 941 CA ATOM 942 CB ATOM 943 CG ATOM 944 CD ATOM 945 NE ATOM 946 CZ ATOM 947 NH ATOM 948 NH ATOM 949 C ATOM 950 0 ATOM 951 N ATOM 951 N ATOM 952 CA ATOM 953 CB ATOM 955 CG ATOM 956 CD ATOM 957 C ATOM 958 0 ATOM 959 N ATOM 960 CD ATOM 960 CD ATOM 961 CA ATOM 963 CC ATOM 963 CC ATOM 965 CD ATOM 965 CD ATOM 966 N ATOM 967 CA ATOM 968 CT ATOM 968 CT ATOM 968 CT ATOM 969 CC ATOM 961 N ATOM 963 CC ATOM 965 O ATOM 966 N ATOM 967 CA ATOM 968 CT ATOM 969 CC ATOM 970 OI ATOM 971 NI ATOM 972 C ATOM 973 O	ARG 147 ARG 148 A 1LE 148 B 1LE 148	54. 692 51. 428 54. 699 52. 706 53. 594 53. 608 53. 708 53. 924 54. 992 54. 651 55. 677 55. 129 55. 309 54. 754 54. 495 52. 521 53. 644 53. 172 55. 287 51. 638 55. 185 51. 357 55. 992 50. 107 55. 376 48. 821 55. 999 47. 649 57. 415 47. 539 58. 271 46. 812 57. 844 46. 143 59. 546 46. 737 55. 623 52. 483 56. 440 53. 330 55. 066 52. 486 55. 430 53. 484 54. 537 53. 642 56. 879 53. 173 57. 240 52. 014 57. 743 55. 645 59. 148 53. 966 59. 765 55. 356 58. 659 56. 244 59. 421 53. 352 58. 621 53. 489	-2. 782 -2. 079 -2. 630 -4. 107 -4. 455 -3. 528 -5. 660 -0. 579 0. 013 1. 262 1. 963 1. 262 1. 963 2. 363 2. 363 2. 363 2. 363 2. 002 3. 568 4. 555 5. 798 6. 940 5. 427 6. 533 4. 891 5. 664 7. 567 6. 748 8. 900 8. 394 10. 208 10. 208	1. 00 33. 82 1. 00 32. 54 1. 00 33. 18 1. 00 33. 14 1. 00 32. 11 1. 00 32. 13 1. 00 32. 26 1. 00 32. 38 1. 00 30. 84 1. 00 29. 94 1. 00 31. 91 1. 00 33. 35 1. 00 34. 66 1. 00 37. 64 1. 00 39. 76 1. 00 40. 68 1. 00 39. 79 1. 00 28. 99 1. 00 29. 74 1. 00 26. 79 1. 00 25. 21 1. 00 24. 62 1. 00 24. 87 1. 00 24. 87 1. 00 24. 99 1. 00 25. 52 1. 00 30. 82 1. 00 35. 16 1. 00 36. 52 1. 00 36. 52	A A A A A A A A A A A A A A A A A A A	NCCCCOOCONCCCCNCNNCONCCCCCCONCCCCONCCCCONCON
ATOM 974 N ATOM 975 C ATOM 976 C ATOM 977 C ATOM 978 O	ASN 151 A ASN 151		10. 208 11. 154 10. 877 11. 048 10. 219			

					F I	G. 4	- 22			(Cont	inued)
ATOM	1029	CG	TRP	157	43. 995		9. 599	1.00 20.88	Α	С	
ATOM	1030	CD2	TRP	157	44.315	53.800	8.364	1.00 18.96	Α	C	
ATOM	1031	CE2	TRP	157	44. 843		8.686	1.00 19.67	Α	С	
ATOM	1032	CE3		157	44. 208		7.019	1.00 17.93	A	C	
ATOM	1033	CD1		157	44. 328		10.592	1.00 20.82	A	C	
ATOM	1034	NE1		157	44. 838		10.052	1.00 21.01	A	N	
ATOM	1035	CZ2		157	45. 265		7. 708	1.00 19.12	A	C	
ATOM	1036	CZ3		157	44.627		6.046	1.00 19.76	A	C	
ATOM	1037	CH2		157	45. 149		6. 397	1.00 19.30	A	C	
ATOM	1038	C	TRP	157	43.650		9.801	1.00 23.03	A	C	
ATOM	1039	0	TRP	157	43. 750		10.843	1.00 25.03	A	0	
ATOM	1040	N	SER	158			8. 784	1.00 23.17	A	N	
ATOM	1041	CA	SER	158	42.064		8. 889	1.00 23.44	A	C	
ATOM	1042	CB	SER	158	41.667		7.502	1.00 22.82	A	C	
ATOM	1043	0G	SER	158	41.208		6.679	1.00 23.84	A	0	
ATOM	1044	C	SER	158	40.845		9.678	1.00 23.86	A	C	
ATOM	1045	0	SER	158	40.613		9. 781	1.00 24.35	A	0	
ATOM	1046	N	PRO	159	40.056		10. 247	1.00 24.17	A	N	
ATOM	1047	CD	PRO	159	40.136		10.114	1.00 24.24	A	C	
ATOM	1048	CA	PRO	159	38. 876		11.029	1.00 23.40	A	C	
ATOM	1049	CB	PRO	159	38. 270		11.419 11.353	1.00 23.45 1.00 24.19	A	C C	
ATOM	1050	CG	PRO	159	39. 4 27 37. 901		10. 224	1.00 24.19	A	Č	
ATOM	1051 1052	C 0	PRO PRO	159 159	37. 191	58. 248	10. 224	1.00 23.30	A A	Õ	
ATOM ATOM	1052	N	VAL	160	37. 137		8. 919	1.00 25.28	A	N	
ATOM	1053	CA	VAL	160	36. 977		8.014	1.00 23.28	A	C	
ATOM	1055	CB	VAL	160	35. 784		7. 689	1.00 24.54	A	č	
ATOM	1056		VAL	160	35.066		6. 449	1.00 26.50	A	č	
ATOM	1057		VAL	160	34. 834		8. 875	1.00 26.15	A	č	
ATOM	1058	C	VAL	160	37.679		6. 730	1.00 23.78	A	č	
ATOM	1059	ŏ	VAL	160	38. 570		6. 245	1.00 24.51	Ä	Ŏ	
ATOM	1060	Ň	GLY	161	37. 268		6. 181	1.00 24.05	Ā	N	
ATOM	1061	ĊA	GLY	161	37.876		4.962	1.00 22.93	A	C	
ATOM	1062	C	GLY	161	39.121		5. 286	1.00 23.87	Α	С	
ATOM	1063	0	GLY	161	39.144		6.269	1.00 24.24	Α	0	
ATOM	1064	N	HIS	162	40.164		4.476	1.00 25.01	Α	N	
ATOM	1065	CA	HIS	162	41.423	3 55. 239	4.695	1.00 25.86	Α	С	
ATOM	1066	CB	HIS	162	41.419	3 53.923	3.920	1.00 26.04	Α	С	
ATOM	1067	CG	HIS	162	41.075		2. 475	1.00 27.52	Α	C	
ATOM	1068	CD2	HIS	162	41.614		1.515	1.00 27.58	Α	C	
ATOM	1069		HIS	162	40. 039		1.874	1.00 27.77	Α	N	
ATOM	1070		HIS	162	39. 956		0.606	1.00 28.51	A	C	
ATOM	1071		HIS	162	40. 900		0. 363	1.00 28.82	A	N	
ATOM	1072	C	HIS	162	42.660		4. 305	1.00 25.44	A	C	
ATOM	1073	0	HIS	162	43. 636		3. 794	1.00 24.38	A	0	
ATOM	1074	N	LYS	163	42.609		4. 527	1.00 24.47	A	N	
ATOM	1075	CA	LYS	163	43. 751		4. 224	1.00 23.45	A	C	
ATOM	1076	CB	LYS	163	43. 372		4. 273	1.00 21.75	A	C	
ATOM	1077	CG	LYS	163	42. 528	3 60.216	3. 130	1.00 21.55	A	С	

									(Continued)
				FIG	. 4 -	23			
ATOM	1078	CD LYS	163	42. 281 6	1.706	3. 335	1.00 20.23	Α	С
ATOM	1079	CE LYS	163		2.316	2.228	1.00 18.07	Α	С
ATOM	1080	NZ LYS	163		3.778	2.422	1.00 20.95	A	Ŋ
ATOM	1081	C LYS	163		7. 961	5.309	1.00 23.44	A	C
ATOM	1082	0 LYS	163		7.600	6.433	1.00 23.42	A	0
ATOM	1083	N LEU	164		8. 146	4. 979	1.00 23.11	A	N
ATOM	1084	CA LEU	164		7. 937	5. 950	1.00 23.65	A	C
ATOM	1085	CB LEU	164		6. 773	5. 524	1. 00 24. 35	A _.	C
ATOM	1086	CG LEU	164		5. 351	5.848	1.00 25.57	A	C
ATOM	1087	CD1 LEU	164		4. 349	5. 219	1.00 25.59	A	C
ATOM	1088	CD2 LEU	164		5. 162	7.359	1.00 25.62	A	C C
ATOM	1089	C LEU	164		9.182		1.00 23.21	A	0
ATOM	1090	0 LEU	164		9. 943	5.177	1.00 24.34 1.00 21.88	A A	N N
ATOM	1091	N ALA	165		9. 383	7. 335 7. 649	1.00 21.00	A A	C
ATOM	1092	CA ALA	165		i0. 508 i1. 583	8.376	1.00 21.38	A	C
ATOM	1093	CB ALA	165		i9. 953	8. 545	1.00 21.77	A	Č
ATOM	1094 1095	C ALA O ALA	165 165		i9. 285	9.537	1.00 22.01	A	Ö
ATOM ATOM	1095	O ALA N TYR	166		io. 208	8. 201	1.00 22.02	A	N
ATOM	1090	CA TYR	166		i9. 697	9.024	1.00 21.73	Ä	č
ATOM	1098	CB TYR	166		8. 319	8. 520	1.00 22.38	Ä	č
ATOM	1099	CG TYR	166		8. 315	7. 141	1.00 22.11	Ä	Č
ATOM	1100	CD1 TYR	166		8. 661	6.964	1.00 21.28	Ä	Č
ATOM	1101	CE1 TYR	166		8. 638	5. 704	1.00 22.05	A	Č
ATOM	1102	CD2 TYR	166		7. 949	6.015	1.00 20.67	A	Ċ
ATOM	1103	CE2 TYR	166		7. 923	4.753	1.00 20.02	Α	С
ATOM	1104	CZ TYR	166		8. 268	4.603	1.00 21.75	Α	С
ATOM	1105	OH TYR	166		8. 252	3.352	1.00 20.77	Α	0
ATOM	1106	C TYR	166	53.927	60.643	9.057	1.00 21.64	A	С
ATOM	1107	0 TYR	166		61.464	8. 157	1.00 21.61	A	0
ATOM	1108	n val	167		30. 529	10.111	1.00 20.28	A	N
ATOM	1109	CA VAL	167		31. 371	10. 264	1.00 19.16	A	C
ATOM	1110	CB VAL	167		52. 011	11.644	1.00 19.56	A	C
ATOM	1111	CG1 VAL	167		52. 984	11.731	1.00 18.58	A	C
ATOM	1112	CG2 VAL	167		32. 713	11.916	1.00 18.36	A	C
ATOM	1113	C VAL	167		50. 537		1.00 20.06	A	C
		0 VAL					1.00 21.80	A	
ATOM	1115	N TRP	168		31.023	9. 233	1.00 19.65	A	N
ATOM	1116	CA TRP	168		30. 320	8.964	1.00 19.61	A	C
ATOM	1117	CB TRP	168		59. 558	7.646	1.00 20.07	A	C
ATOM	1118	CG TRP	168		58. 772	7. 353	1.00 23.12 1.00 21.38	A A	C C
ATOM	1119	CD2 TRP	168 168		59. 011 58. 061	6.300 6.436	1.00 21.58	A	C
ATOM	1120 1121	CE2 TRP CE3 TRP	168		59. 936	5. 256	1.00 21.74	A	Č
ATOM ATOM	1121	CD1 TRP	168		57. 712	8. 066	1.00 21.74	A	C
ATOM	1123	NE1 TRP	168		57. 281	7. 521	1.00 21.54	Ä	N
ATOM	1123	CZ2 TRP	168		58. 012	5. 563	1.00 23.71	Ä	Ċ
ATOM	1125	CZ3 TRP	168		59. 889	4. 386	1.00 23.21	Ä	č
ATOM	1126	CH2 TRP	168		58. 934	4.546	1.00 22.74	Ä	č
VIOI	1140	OHE HA	100	00.707	,u, Jur	1. 0 10	2.00 00.11	••	•

										(Continued)
					FΙ	G. 4	- 26			
ATOM	1225	CD1	IRII	180	46. 604	56. 359	-5. 856	1.00 23.58	Α	С
ATOM	1226	CD2		180	48. 224	54. 503	-6. 328	1.00 22.86	A	Č
ATOM	1227		LEU	180	50. 938	55.996	-3. 391	1.00 25.78	Ā	Ċ
ATOM	1228		LEU	180	51. 185	55. 883	-2. 185	1.00 23.62	A	Ō
ATOM	1229		PRO	181	51.669	56. 789	-4.194	1.00 24.96	A	N
ATOM	1230		PRO	181	51.687	56.842	-5.667	1.00 23.41	Α	C
ATOM	1231		PRO	181	52.766	57.580	-3.634	1.00 23.35	Α	C
ATOM	1232	CB	PRO	181	53.403		-4.870	1.00 22.16	Α	C
ATOM	1233		PR0	181	53. 124		-5.944	1.00 22.72	Α	C
ATOM	1234	C	PRO	181	52.216	58.613	-2.667	1.00 22.15	Α	C
ATOM	1235	0	PRO	181	51.144		-2.880	1.00 21.88	Α	0
ATOM	1236	N	SER	182	52.954		-1.601	1.00 21.65	A	N
ATOM	1237	CA	SER	182	52.516	59.829	-0.620	1.00 20.50	A	C
ATOM	1238	CB	SER	182	52.999		0. 765	1.00 22.61	A	C
ATOM	1239	0G	SER	182	54. 408		0.806	1.00 23.55	A	0
ATOM	1240	C	SER	182	53. 034		-0.947	1.00 19.05	A	C
ATOM	1241	0	SER	182	54.003		-1.687	1.00 17.74	A	0
ATOM	1242	N	TYR	183	52.366	62. 233	-0.402	1.00 17.87	A	N
ATOM	1243	CA	TYR	183	52. 786	63.606	-0.611	1.00 15.17 1.00 12.09	A	C.
ATOM	1244	CB	TYR	183	51.595 50.676	64. 523 64. 028	-0.832 -1.905	1.00 12.09	A A	C
ATOM	1245	CG	TYR TYR	183 183	49. 729		-1.625	1.00 12.34	A	C
ATOM ATOM	1246 1247		TYR	183	48. 916		-2. 610	1.00 11.95	A	C
ATOM	1248		TYR	183	50. 782		-3. 214	1.00 9.42	A	Č
ATOM	1249		TYR	183	49. 961	63. 990	-4. 218	1.00 10.27	A	č
ATOM	1250	CZ	TYR	183	49. 032		-3. 903	1.00 10.59	A	č
ATOM	1251	OH	TYR	183	48. 205		-4. 867	1.00 14.71	Ä	Ö
ATOM	1252	C	TYR	183	53. 532		0.617	1.00 15.72	A	Ċ
ATOM	1253	Ŏ	TYR	183	53. 208		1.740	1.00 17.69	A	0
ATOM	1254	N	ARG	184	54. 540		0.386	1.00 14.64	Α	N
ATOM	1255	CA	ARG	184	55. 342		1.452	1.00 14.10	Α	С .
ATOM	1256	CB	ARG	184	56. 786	65.593	0.970	1.00 16.84	Α	C
ATOM	1257	CG	ARG	184	57. 725		1.989	1.00 20.48	Α	С
ATOM	1258	CD	ARG	184	59. 170		1.629	1.00 20.61	A	C
ATOM	1259	NE	ARG	184	60.095		2. 598	1.00 20.21	A	N
ATOM	1260	CZ	ARG	184	61.407		2. 583	1.00 19.46	A	Ç
ATOM	1261			184				1.00 17.13	A	
ATOM	1262		ARG	184	62. 170		3. 506	1.00 20.35	A	N
ATOM	1263	C	ARG	184	54. 736		1.820	1.00 14.10	A	C
ATOM	1264	0	ARG	184	54. 569		0.972	1.00 14.71	A	0 N
ATOM	1265	N	ILE	185	54. 390 53. 804		3. 089 3. 572	1.00 15.27 1.00 14.44	A A	N C
ATOM	1266	CA CB	ILE	185 185	52. 786		4. 692	1.00 14.44	A	Č
ATOM ATOM	1267 1268		ILE	185	52. 760 52. 091	69.175	5. 115	1.00 10.20	Ä	Č
ATOM	1269		ILE	185	51. 770		4. 202	1.00 14.78	Ä	Č
ATOM	1270		ILE	185	51.021	67. 250	2. 947	1.00 12.00	A	č
ATOM	1271	C	ILE	185	54. 847		4. 091	1.00 14.33	Ä	č
ATOM	1272	ŏ	ILE	185	54. 647		3. 994	1.00 14.95	Ä	Ö
ATOM	1273	Ň	THR	186	55. 950		4. 646	1.00 14.38	A	N
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				FΙ	G. 4	- 27			(Continued)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	1277 CG2 1278 C 1279 O 1280 N 1281 CA 1282 CB 1283 CG 1284 CD2 1285 CE2 1286 CE3 1287 CD1 1288 NE1 1289 CZ2 1291 CH2 1292 C 1293 O 1294 N 1295 CA 1296 CB 1297 OG1 1298 CG2 1299 C 1300 O 1301 N 1302 CA 1303 C 1304 O 1305 N 1306 CA 1307 CB 1308 CG 1309 CD 1310 CE 1311 NZ 1312 C 1313 O 1314 N	TRP	186 186 186 186 186 187 187 187 187 187 187 187 187 187 187	56. 995 57. 051 57. 308 55. 734 58. 384 58. 643 59. 055 60. 843 60. 392 59. 055 59. 093 57. 829 61. 165 60. 392 56. 692 56. 758 61. 607 62. 804 61. 077 61. 892 61. 122 59. 855 60. 398 61. 122 59. 855 60. 189 61. 189 62. 384 64. 196 65. 612 66. 189 67. 679 68. 181 69. 207 65. 384 66. 426	69. 555 69. 549 68. 218 70. 069. 190 68. 055 70. 174 70. 020 70. 734 69. 949 68. 954 70. 405 69. 149 68. 549 68. 616 70. 074 69. 185 70. 620 70. 725 71. 605 72. 737 72. 253 73. 920 70. 642 71. 016 68. 421 68. 685 68. 612 69. 512 69. 528 70. 997 71. 663 69. 512 69. 512 69. 528 70. 620 70. 725 71. 016 69. 512 69. 512 69. 512 69. 513 69. 513 6	5. 169 6. 717 7. 181 7. 323 4. 663 4. 262 4. 696 4. 253 2. 915 1. 736 1. 234 0. 135 1. 606 0. 941 -0. 020 -0. 597 0. 881 -0. 211 5. 292 5. 053 6. 449 7. 493 8. 180 8. 587 7. 232 9. 415 8. 552 9. 415 8. 552 9. 782 8. 881 11. 004 11. 346 11. 264 11. 346 11. 273 12. 747 13. 737 12. 811	1. 00 15. 05 1. 00 15. 72 1. 00 18. 48 1. 00 13. 92 1. 00 17. 06 1. 00 19. 33 1. 00 18. 28 1. 00 16. 04 1. 00 13. 96 1. 00 15. 37 1. 00 15. 37 1. 00 15. 22 1. 00 12. 92 1. 00 12. 92 1. 00 15. 60 1. 00 17. 91 1. 00 15. 71 1. 00 15. 71 1. 00 15. 71 1. 00 19. 54 1. 00 13. 19 1. 00 11. 35 1. 00 11. 04 1. 00 9. 11 1. 00 9. 11 1. 00 7. 35 1. 00 12. 10 1. 00 9. 49 1. 01 12. 10 1. 00 9. 49 1. 01 15. 86 1. 00 17. 65 1. 00 17. 28 1. 00 17. 65 1. 00 17. 28 1. 00 17. 65 1. 00 17. 28 1. 00 17. 65 1. 00 17. 28 1. 00 17. 65 1. 00 17. 65 1. 00 17. 65 1. 00 18. 87 1. 00 20. 03 1. 00 22. 58 1. 00 27. 62 1. 00 31. 27 1. 00 35. 57 1. 00 18. 55 1. 00 18. 41 1. 00 19. 79 1. 00 21. 70	A A A A A A A A A A A A A A A A A A A	CCOCCONCCCCCNCCCONCCCONCCONCCCONCCCNCON
ATOM ATOM ATOM ATOM ATOM ATOM ATOM	1315 CA 1316 CB 1317 CG 1318 CD 1319 OE1 1320 OE2 1321 C	GLU GLU GLU GLU GLU GLU GLU	191 191 191 191 191 191	66. 674 67. 796 67. 894 69. 018 68. 970 69. 952 67. 015	65. 661 64. 653 63. 598 62. 605 61. 497 62. 932 66. 583	14. 062 13. 851 14. 937 14. 689 15. 262 13. 929 15. 236	1.00 21.70 1.00 23.41 1.00 29.95 1.00 30.89 1.00 33.70 1.00 33.21 1.00 21.53	A A A A A	N C C C O O C
ATOM	1322 0	GLU	191	67.930	67. 397	15. 156	1.00 22.21	A	U

FIG. 4 - 28 ATOM 1323 N ASP 192 66.262 66.451 16.320 1.00 21.17 A N ATOM 1324 CA ASP 192 66.470 67.246 17.525 1.00 22.27 A C ATOM 1325 CB ASP 192 67.810 66.880 18.182 1.00 23.92 A C ATOM 1326 CG ASP 192 67.922 65.400 18.510 1.00 25.20 A C ATOM 1327 OD1 ASP 192 66.891 64.775 18.850 1.00 25.70 A O ATOM 1328 OD2 ASP 192 69.049 64.866 18.438 1.00 26.25 A O ATOM 1329 C ASP 192 66.425 68.759 17.341 1.00 21.93 A C					(Continued))
ATOM 1324 CA ASP 192 66. 470 67. 246 17. 525 1. 00 22. 27 A C ATOM 1325 CB ASP 192 67. 810 66. 880 18. 182 1. 00 23. 92 A C ATOM 1326 CG ASP 192 67. 922 65. 400 18. 510 1. 00 25. 20 A C ATOM 1327 OD1 ASP 192 66. 891 64. 775 18. 850 1. 00 25. 70 A O ATOM 1328 OD2 ASP 192 69. 049 64. 866 18. 438 1. 00 26. 25 A O ATOM 1329 C. ASP 192 66. 425 68. 759 17. 341 1. 00 21. 93 A C	••	FΙ	G. 4 - 28			
ATOM 1330 O ASP 192 66.998 69.489 18.145 1.00 22.788 A O ATOM 1331 N ILE 193 65.748 69.242 16.304 1.00 21.66 A N ATOM 1332 CA ILE 193 65.685 70.684 16.071 1.00 20.08 A C ATOM 1333 CB ILE 193 66.707 72.567 14.677 1.00 18.91 A C ATOM 1335 CGI ILE 193 66.570 72.567 14.677 1.00 18.91 A C ATOM 1335 CGI ILE 193 68.142 70.889 15.624 1.00 22.58 A C ATOM 1335 CGI ILE 193 69.263 71.198 14.671 1.00 26.43 A C ATOM 1337 C ILE 193 64.318 71.172 15.615 1.00 19.15 A C ATOM 1338 0 ILE 193 64.318 71.172 15.615 1.00 19.15 A C ATOM 1339 N ILE 194 63.814 70.594 14.534 1.00 19.04 A N ATOM 1340 CA ILB 194 62.506 70.967 14.021 1.00 17.41 A C ATOM 1341 CB ILE 194 62.506 70.967 14.021 1.00 17.41 A C ATOM 1341 CB ILE 194 63.814 70.594 14.534 1.00 19.04 A N C ATOM 1343 CGI ILE 194 63.551 72.750 12.553 1.00 16.97 A C C ATOM 1345 CGI ILE 194 63.551 72.750 12.553 1.00 18.89 A C ATOM 1345 CGI ILE 194 63.551 72.750 12.553 1.00 18.89 A C C ATOM 1345 CGI ILE 194 63.561 72.750 12.553 1.00 16.97 A C C ATOM 1345 CGI ILE 194 63.561 72.750 12.553 1.00 18.89 A C C ATOM 1345 CGI ILE 194 63.561 72.750 12.553 1.00 16.97 A C C ATOM 1345 CGI ILE 194 63.561 72.750 12.553 1.00 16.97 A C C ATOM 1345 CGI ILE 194 63.663 69.702 13.969 1.00 18.22 A C ATOM 1345 CGI ILE 194 61.663 69.702 13.969 1.00 18.22 A C ATOM 1345 CGI ILE 194 62.606 68.713 13.349 1.00 17.31 A N ATOM 1345 CGI ILE 194 62.606 66 87.71 1.00 17.31 A N ATOM 1345 CGI ITE 194 62.606 66 87.71 1.00 17.31 A N ATOM 1345 CGI TYR 195 60.511 69.726 14.642 1.00 17.31 A N ATOM 1345 CGI TYR 195 60.510 69.726 14.642 1.00 17.31 A N ATOM 1345 CGI TYR 195 60.560 67.776 16.893 1.00 16.19 A C ATOM 1350 CG TYR 195 60.560 67.776 16.893 1.00 16.19 A C ATOM 1351 CDI TYR 195 61.427 68.802 17.286 1.00 18.28 A C ATOM 1355 CG TYR 195 60.560 67.776 16.893 1.00 17.58 A C ATOM 1355 CG TYR 195 60.560 67.776 16.893 1.00 17.41 A C ATOM 1356 CG ANN 196 57.591 70.133 10.489 1.00 16.19 A C ATOM 1356 CG ANN 196 56.575 86.694 67.776 18.624 1.00 17.41 A C ATOM 1366 O ANN 196 56.575 86.604 67.776 18.802 17.00 15.26 A N ATOM 1366 O ANN 19	ATOM 1323 N AN ATOM 1324 CA ATOM 1325 CB ATOM 1326 CG A ATOM 1327 OD1 A ATOM 1328 OD2 A ATOM 1329 C A ATOM 1330 O A ATOM 1331 N I ATOM 1331 N I ATOM 1334 CG2 I ATOM 1335 CG1 I ATOM 1336 CD1 I ATOM 1337 C I ATOM 1338 O I ATOM 1339 N I ATOM 1340 CA I ATOM 1341 CB I ATOM 1342 CG2 I ATOM 1342 CG2 I ATOM 1343 CG1 I ATOM 1344 CD1 I ATOM 1345 C I ATOM 1345 C I ATOM 1346 O I ATOM 1347 N I ATOM 1346 O I ATOM 1347 N I ATOM 1348 CA I ATOM 1349 CB I ATOM 1349 CB I ATOM 1346 O I ATOM 1347 N I ATOM 1348 CA I ATOM 1349 CB I ATOM 1349 CB I ATOM 1350 CG I ATOM 1350 CG I ATOM 1351 CD1 I ATOM 1352 CE1 I ATOM 1353 CD2 I ATOM 1354 CE2 I ATOM 1355 CZ ATOM 1355 CZ ATOM 1356 OH ATOM 1357 C ATOM 1357 C ATOM 1357 C ATOM 1358 O ATOM 1359 N ATOM 1356 CA ATOM 1361 CB ATOM 1363 OD1 ATOM 1363 OD1 ATOM 1365 C ATOM 1366 O ATOM 1367 N ATOM 1366 O ATOM 1367 N ATOM 1368 CA ATOM 1366 O ATOM 1367 N ATOM 1368 CA ATOM 1366 O ATOM 1367 N ATOM 1368 CA ATOM 1366 O ATOM 1367 N ATOM 1368 CA ATOM 1368 CA ATOM 1369 C	ASP 192 66. 262 ASP 192 66. 470 ASP 192 67. 810 ASP 192 67. 922 ASP 192 66. 891 ASP 192 69. 049 ASP 192 66. 425 ASP 192 66. 998 ILE 193 65. 685 ILE 193 65. 685 ILE 193 66. 570 ILE 193 68. 142 ILE 193 68. 142 ILE 193 63. 736 ILE 194 63. 814 ILE 194 62. 506 ILE 194 63. 551 ILE 194 63. 551 ILE 194 63. 63. 718 ILE 194 63. 63. 718 ILE 194 63. 551 ILE 194 63. 551 ILE 194 63. 551 ILE 195 60. 560 TYR 195 59. 338 TYR 195 59. 338 TYR 195 60. 560 TYR 195 60. 560 TYR 195 62. 485 TYR 195 62. 485 TYR 195 63. 725 TYR 195 63. 725 TYR 195 63. 725 TYR 195 65. 664 ASN 196 57. 591 ASN 196 56. 050 GLY 197 54. 522 GLY 197 53. 622 GLY 197 53. 623 GLY 197 53. 623 GLY 197 53. 623 GLY 197 53. 623	66. 451	1.00 22.27 1.00 23.92 1.00 25.20 1.00 25.70 1.00 26.25 1.00 21.93 1.00 22.78 1.00 21.66 1.00 20.08 1.00 20.73 1.00 18.91 1.00 22.58 1.00 26.43 1.00 19.15 1.00 19.55 1.00 19.55 1.00 19.697 1.00 18.89 1.00 16.97 1.00 18.89 1.00 16.97 1.00 18.22 1.00 17.31 1.00 18.22 1.00 17.31 1.00 18.22 1.00 17.31 1.00 18.28 1.00 15.10 1.00 17.58 1.00 18.28 1.00 15.10 1.00 15.14 1.00 15.26 1.00 15.27 1.00 12.88 1.00 15.27 1.00 12.88 1.00 15.27 1.00 12.88 1.00 15.27 1.00 12.88 1.00 15.27 1.00 12.88 1.00 15.27 1.00 12.88 1.00 15.14 1.00 15.27 1.00 15.85 1.00 15.27 1.00 15.85 1.00 15.27 1.00 15.85 1.00 15.55	A A A A A A A A A A A A A A A A A A A	

					T2 T	C 1.	- 20			(Contin	ued)
, mc	10-0	0.1	** 5	100		G. 4		1.00 16.59	A	С	
ATOM	1372		ILE	198	55. 378	65.097 63.991	16. 298 16. 011	1.00 10.33	A	č	
ATOM	1373		ILE	198	56. 425 55. 874	63.013	14. 987	1.00 18.21	A	č	
ATOM	1374	CG2		198 198	57. 724	64.602	15. 494	1.00 17.86	Ä	č	
ATOM ATOM	1375 1376	CG1 CD1		198	58. 798	63. 565	15. 214	1.00 19.35	A	Č	
ATOM	1377		ILE	198	55. 946	66.057	17. 318	1.00 15.95	Ä	Ċ	
ATOM	1378		ILE	198	56.507	67.091	16.966	1.00 17.63	· A	0	
ATOM	1379		THR	199	55. 809	65.700	18.583	1.00 15.42	Α	N	
ATOM	1380		THR	199	56. 264	66.547	19.672	1.00 16.68	Α	С	
ATOM	1381		THR	199	55. 374	66.316	20.908	1.00 17.40	Α	С	
ATOM	1382		THR	199	55.462	64.944	21.301	1.00 18.82	Α	0	
ATOM	1383	CG2	THR	199	53. 924	66.619	20. 583	1.00 15.72	A	C	
ATOM	1384		THR	199	57.716	66.334	20.076	1.00 16.00	A	C	
ATOM	1385		THR	199	58. 317	65. 325	19.734	1.00 16.12	A	0	
ATOM	1386		ASP	200	58. 276	67. 301	20.801	1.00 16.87	A	N	
ATOM	1387		ASP	200	59.649	67. 193	21. 289	1.00 15.49	A	C	
ATOM	1388		ASP	200	60. 315	68.576	21.418	1.00 14.82	A A	C C	
ATOM	1389		ASP	200	59. 681	69. 446 69. 190	22. 491 22. 873	1.00 17.16 1.00 16.41	A	ŏ	
ATOM	1390	0D1 0D2		200 200	58. 517 60. 348		22. 945	1.00 15.41	A	Ŏ	
ATOM ATOM	1391 1392	C	ASP	200	59.496		22.641	1.00 15.54	A	Č	
ATOM	1393		ASP	200	58. 388		22. 999	1.00 17.01	A	ŏ	
ATOM	1394	N	TRP	201	60. 581	66. 381	23. 395	1.00 15.10	A	Ň	
ATOM	1395	CA	TRP	201	60. 504		24.672	1.00 13.14	A	C	
ATOM	1396	CB	TRP	201	61.885		25.326	1.00 14.90	Α	С	
ATOM	1397	CG	TRP	201	61.905		26.510	1.00 15.25	Α	C	
ATOM	1398	CD2	TRP	201	61.412	64. 953	27.828	1.00 13.65	Α	C	
ATOM	1399	CE2		201	61.500		28.564	1.00 13.52	A	C	
ATOM	1400	CE3		201	60. 902		28. 456	1.00 11.78	A	C	
ATOM	1401	CD1		201	62. 269		26. 507	1.00 13.81	A	C	
ATOM	1402	NE1		201	62.025		27. 733	1.00 13.64	A	N	
ATOM	1403	CZ2		201	61.096		29.897	1.00 14.03	A	C	
ATOM	1404	CZ3		201	60. 502		29. 778	1.00 12.04	A	C	
ATOM	1405	CH2 C	TRP TRP	201 201	60. 601 59. 529		30. 486 25. 662	1.00 14.87 1.00 14.42	A A	C C	
ATOM	1406 1407		TRP	201	58. 635		26. 175	1.00 14.42	A	ŏ	
ATOM ATOM	1408	N	VAL	202	59. 691	67.615	25. 931	1.00 15.14	Ä	Ň	
ATOM	1409	CA	VAL	202	58. 830		26.911	1.00 14.23	Ä	Ċ	
ATOM	1410	CB	VAL	202	59. 402		27. 330	1.00 12.99	Ä	Č	
ATOM	1411	CG1		202	59.010		26. 322	1.00 11.02	A	C	
ATOM	1412	CG2		202	58.947		28. 753	1.00 8.71	Α	С	
ATOM	1413	C	VAL	202	57. 365		26.518	1.00 15.76	Α	С	
ATOM	1414	0	VAL	202	56. 497	68. 404	27. 391	1.00 18.74	Α	0	
ATOM	1415	N	TYR	203	57.072		25. 226	1.00 15.58	A	N	
ATOM	1416	CA	TYR	203	55. 676		24. 805	1.00 14.25	A	C	
ATOM	1417	CB	TYR	203	55. 556		23. 354	1.00 14.63	A	C	
ATOM	1418	CG	TYR	203	55. 227		23. 227	1.00 12.35	A	C	
ATOM	1419		TYR	203	56. 231		23. 193	1.00 11.91	A	C C	
ATOM	1420	CEI	TYR	203	55. 920	72.867	23. 108	1.00 11.20	A	C	

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ATOM	1470	С	PHE	208	50.082	65.163	25.506	1.00 26.13	Α	C
ATOM	1471		PHE	208	49. 215	64.471	24.985	1.00 27.79	Α	0
ATOM	1472	Ň	SER	209	50. 918	64.687	26, 421	1.00 26.62	A	N
	1473	CA	SER	209	50. 852	63. 293	26.848	1.00 25.74	Α	С
ATOM					49. 645	63.059	27. 743	1.00 24.80	Ä	С
ATOM	1474	CB	SER	209			29. 014	1.00 29.47	Ä	Ŏ
ATOM	1475	0G	SER	209	49.871	63.629				Č
ATOM	1476	C	SER	209	50.773	62.377	25. 642	1.00 25.50	A	
ATOM	1477	0	SER	209	50. 278	61.249	25.716	1.00 25.72	A	0
ATOM	1478	N	ALA	210	51.272	62.875	24.524	1.00 23.72	A	N
ATOM	1479	CA	ALA	210	51.263	62.112	23. 299	1.00 22.80	A	C
ATOM	1480	CB	ALA	210	49. 977	62.364	22.530	1.00 20.62	Α	C
ATOM	1481	C	ALA	210	52.455	62.560	22.492	1.00 21.87	Α	C
ATOM	1482	ŏ	ALA	210	52. 986	63.644	22.703	1.00 22.09	Α	0
			TYR	211	52. 863	61.719	21.558	1.00 21.57	Ā	N
ATOM	1483	N				62.009	20.718	1.00 21.42	Ä	Ċ
ATOM	1484	CA	TYR	211	54.000			1.00 19.58	Ä	č
ATOM	1485	CB	TYR	211	54. 725	60.711	20.405			Č
ATOM	1486	CG	TYR	211	55. 921	60.870	19.528	1.00 16.81	A	
ATOM	1487	CD1	TYR	211	56.853	61.870	19.770	1.00 16.07	A	C
ATOM	1488	CE1	TYR	211	58. 002	61.971	19.001	1.00 18.18	A	C
ATOM	1489	CD2	TYR	211	56.`160	59.976	18.489	1.00 17.91	A	C
ATOM	1490			211	57. 306	60.065	17.716	1.00 18.80	A	C
ATOM	1491	CZ	TYR	211	58. 221	61.063	17.979	1.00 18.36	Α	С
ATOM	1492	OH	TYR	211	59. 360	61.149	17.224	1.00 23.65	Α	0
	1493	C	TYR	211	53. 588	62. 689	19. 428	1.00 22.96	A	Č
ATOM				211	54. 365	63. 443	18. 837	1.00 25.79	Ä	ŏ
ATOM	1494	0	TYR				18. 983	1.00 20.15	A	N
ATOM	1495	N	SER	212	52. 365	62. 433				
ATOM	1496	CA	SER	212	51.918	63.033	17.746	1.00 19.56	A	C
ATOM	1497	CB	SER	212	50. 835	62. 175	17.090	1.00 20.97	A	C
ATOM	1498	0G	SER	212	49.635	62. 208	17.829	1.00 21.79	A	0
ATOM	1499	C	SER	212	51.397	64.439	17. 959	1.00 18.50	A	C
ATOM	1500	0	SER	212	50. 933	64. 789	19.040	1.00 16.31	A	0
ATOM	1501	N	ALA	213	51.493	65. 236	16.901	1.00 17.84	A	N
ATOM	1502	CA	ALA	213	51.036	66.610	16.903	1.00 16.02	A	C
ATOM	1503	CB	ALA	213	52. 193	67.548	17.224	1.00 14.16	A	C
ATOM	1504	C	ALA	213	50. 429	66.935	15.526	1.00 15.57	Α	C
ATOM	1505	ŏ	ALA	213	50. 857	67. 862	14. 833	1.00 13.25	A	Ŏ
			LEU	214	49. 448	66. 132	15. 129	1.00 14.75	Ä	Ň
ATOM	1506	N						1.00 14.10	A	C
ATOM	1507	CA	LEU	214	48. 734	66. 339	13.874			Č
ATOM	1508	CB	LEU	214	49. 353	65.517	12. 735	1.00 16.40	A	
ATOM	1509	CG	LEU	214	49. 482	63.999	12.823	1.00 17.01	A	Č
ATOM	1510		LEU	214	48. 135	63.342	12.628	1.00 18.97	A	C
ATOM	1511	CD2	LEU	214	50. 434	63.535	11.742	1.00 16.98	A	C
ATOM	1512	С	LEU	214	47. 273	65.963	14.124	1.00 16.65	A	C
ATOM	1513	Õ	LEU	214	46.966	64.933	14.728	1.00 18.12	Α	0
ATOM	1514	Ň	TRP	215	46. 366	66.811	13.666	1.00 16.16	Α	N
ATOM	1515	ČA	TRP	215	44. 959	66. 590	13.907	1.00 14.69	Ā	C
		CB	TRP	215	44. 471	67.663	14.863	1.00 15.49	Ä	Č
ATOM	1516					67.669	16.145	1.00 17.52	A	č
ATOM	1517	CG	TRP	215	45. 230			1.00 17.32	A	Č
ATOM	1518	CDZ	TRP	215	46. 482	68. 325	16.403	1.00 11.14	V	U

						(Continued)
				FIG. 4-32		(00111111111111111111111111111111111111
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	1520 CE3 1521 CD3 1522 NE3 1523 CZ3 1524 CZ3 1525 CH3 1526 C 1527 O 1528 N 1529 CA 1530 CB 1531 CG 1532 CD 1533 CE 1534 CE	TRP TRP 2 TRP 2 TRP 3 TRP	215 215 215 215 215 215 215 216 216 216 216 216 216 216	46. 852 68. 008 17. 729 1. 00 17. 50 47. 325 69. 149 15. 643 1. 00 18. 21 44. 904 67. 004 17. 289 1. 00 15. 79 45. 873 67. 202 18. 243 1. 00 17. 35 48. 033 68. 485 18. 318 1. 00 18. 06 48. 505 69. 625 16. 228 1. 00 18. 96 48. 844 69. 289 17. 555 1. 00 18. 21 44. 110 66. 605 12. 661 1. 00 15. 55 43. 869 67. 668 12. 090 1. 00 16. 18 43. 646 65. 430 12. 244 1. 00 15. 31 42. 793 65. 330 11. 069 1. 00 16. 40 42. 494 63. 873 10. 739 1. 00 16. 43 43. 549 63. 114 10. 002 1. 00 17. 38 43. 823 63. 169 8. 599 1. 00 17. 01 44. 794 62. 176 8. 320 1. 00 17. 25 43. 340 63. 954 7. 549	A A A A A A A A A A A A A A A A A A A	(Continued) C C C C N C C C C C C C C C C C C C C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	1535 CD 1536 NE 1537 CZ 1538 CZ 1539 CH 1540 C 1541 O 1542 N 1543 CA 1544 CB 1545 OG 1546 C	1 TRP 1 TRP 2 TRP 3 TRP 2 TRP TRP TRP SER SER SER SER SER	216 216 216 216 216 216 217 217 217 217 217	44. 352 62. 125 10. 508 1. 00 18. 55 45. 098 61. 553 9. 501 1. 00 18. 07 45. 286 61. 951 7. 036 1. 00 15. 24 43. 829 63. 729 6. 270 1. 00 17. 06 44. 794 62. 734 6. 027 1. 00 17. 07 41. 461 66. 016 11. 355 1. 00 17. 17 40. 990 66. 005 12. 487 1. 00 18. 00 40. 847 66. 605 10. 334 1. 00 18. 39 39. 552 67. 240 10. 523 1. 00 19. 62 39. 257 68. 225 9. 392 1. 00 20. 31 39. 234 67. 589 8. 133 1. 00 24. 00 38. 528 66. 108 10. 550 1. 00 20. 47	A A A A A A A A A	C N C C C O N C C O C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	1560 NI 1561 C 1562 O	PRO PRO PRO PRO PRO ASN ASN B ASN B ASN B ASN ASN ASN ASN ASN ASN ASN	217 218 218 218 218 218 218 219 219 219 219 219 219 219	38. 814 64. 994 10. 110 1. 00 20. 32 37. 326 66. 369 11. 074 1. 00 20. 82 36. 827 67. 650 11. 598 1. 00 20. 28 36. 285 65. 339 11. 154 1. 00 22. 67 35. 033 66. 148 11. 462 1. 00 21. 68 35. 587 67. 223 12. 353 1. 00 21. 12 36. 123 64. 404 9. 950 1. 00 23. 46 36. 190 63. 183 10. 107 1. 00 25. 13 35. 909 64. 948 8. 756 1. 00 22. 93 35. 756 64. 071 7. 600 1. 00 22. 31 34. 704 64. 622 6. 631 1. 00 22. 48 35. 172 65. 849 5. 903 1. 00 24. 12 36. 373 66. 076 5. 760 1. 00 26. 01 34. 230 66. 640 5. 411 1. 00 26. 27 37. 090 63. 841 6. 871 1. 00 20. 94 38. 184 64. 267 7. 499	A A A A A A A A A A A A A A A A A A A	0 N C C C C C O N C C C O N C O N
ATOM ATOM ATOM ATOM ATOM	1563 N 1564 C/ 1565 C 1566 O 1567 N	GLY GLY GLY GLY THR	220 220 220 220 221	38. 184 64. 267 7. 499 1. 00 18. 33 39. 512 64. 068 6. 941 1. 00 17. 97 40. 035 64. 993 5. 853 1. 00 18. 92 41. 157 64. 801 5. 375 1. 00 20. 28 39. 242 65. 980 5. 447 1. 00 17. 57	A A A A	C C O N

					(Continued)
				FIG. 4-33	(Continued)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	1569 C 1570 C 1571 C 1572 C 1573 C 1574 N 1575 C 1576 C 1577 C 1578 C 1579 C 1580 C 1581 C 1582 C 1583 C 1584 C 1585 N 1586 C 1587 C 1588 C 1588 C) THR	221 221 221 221 221 222 222 222 222 222	39. 654 66. 917 4. 408 1. 00 15. 80 A 38. 540 67. 942 4. 112 1. 00 15. 67 A 37. 410 67. 269 3. 550 1. 00 16. 41 A 39. 019 69. 004 3. 147 1. 00 12. 96 A 40. 903 67. 674 4. 833 1. 00 16. 70 A 41. 884 67. 753 4. 088 1. 00 16. 98 A 40. 864 68. 238 6. 033 1. 00 15. 92 A 41. 999 69. 001 6. 539 1. 00 15. 88 A 41. 508 70. 253 7. 262 1. 00 15. 20 A 40. 939 71. 305 6. 356 1. 00 14. 35 A 39. 569 71. 542 6. 323 1. 00 11. 89 A 41. 782 72. 097 5. 571 1. 00 14. 45 A 39. 046 72. 550 5. 533 1. 00 13. 50 A 41. 269 73. 112 4. 771 1. 00 12. 61 A 39. 897 73. 342 4. 751 1. 00 15. 23 A 42. 907 68. 228 7. 494 1. 00 15. 23 A 42. 907 68. 228 7. 494 1. 00 16. 13 A 42. 467 67. 327 8. 211 1. 00 16. 82 A 44. 187 68. 582 7. 484 1. 00 15. 93 A 45. 159 67. 983 8. 385 1. 00 14. 81 A 46. 199 67. 142 7. 645 1. 00 14. 94 46. 696 65. 773 9. 687 1. 00 11. 99	N C C C
	1589 (1590 (223 223 223	46. 696 65. 773 9. 687 1. 00 11. 99 A 48. 338 65. 830 7. 808 1. 00 11. 50 A 45. 848 69. 162 9. 031 1. 00 16. 80 A	C C C
ATOM ATOM ATOM	1592 (1593 f 1594 (O LEU N ALA CA ALA	223 224 224	46. 398 70. 028 8. 341 1. 00 16. 53 A 45. 790 69. 219 10. 353 1. 00 17. 34 A 46. 420 70. 308 11. 073 1. 00 18. 47 A	N C
ATOM ATOM ATOM ATOM	1596 (1597 (CB ALA C ALA O ALA N TYR	224 224 224 225	47. 596 69. 735 11. 840 1. 00 18. 77 A 47. 587 68. 561 12. 205 1. 00 19. 22 A 48. 614 70. 551 12. 078 1. 00 17. 68 A	C O N
ATOM ATOM ATOM ATOM	1600 (1601 (CA TYR CB TYR CG TYR CD1 TYR	225 225 225 225	49. 764 70. 068 12. 819 1. 00 17. 56 A 50. 726 69. 306 11. 891 1. 00 16. 48 A 51. 273 70. 108 10. 726 1. 00 15. 05 A 50. 551 70. 235 9. 533 1. 00 13. 44 A	C C
ATOM ATOM ATOM ATOM	1603 (1604 (1605 (CE1 TYR CD2 TYR CE2 TYR CZ TYR	225 225 225 225 225	51. 050 70. 968 8. 456 1. 00 9. 19 A 52. 514 70. 740 10. 814 1. 00 14. 42 A 53. 025 71. 476 9. 744 1. 00 14. 09 A 52. 286 71. 583 8. 567 1. 00 14. 11 A	C C C
ATOM ATOM ATOM	1607 (1608 (OH TYR C TYR O TYR	225 225 225	52. 802 72. 292 7. 504 1. 00 14. 49 A 50. 514 71. 182 13. 521 1. 00 17. 79 A 50. 326 72. 359 13. 229 1. 00 19. 91 A	0 C 0
ATOM ATOM ATOM ATOM	1610 1 1611 (1612 (N ALA CA ALA CB ALA C ALA	226 226 226 226	51. 358 70. 796 14. 462 1. 00 17. 65 A 52. 164 71. 748 15. 201 1. 00 17. 74 A 52. 060 71. 472 16. 687 1. 00 18. 89 53. 601 71. 575 14. 740 1. 00 17. 39 A	N C C
ATOM ATOM ATOM	1614 1615	O ALA N GLN CA GLN	226 227 227	53. 966 70. 527 14. 204 1. 00 16. 05 54. 412 72. 606 14. 941 1. 00 17. 45 55. 816 72. 552 14. 555 1. 00 16. 64	0 N

(Continued)

FIG. 4-34 13.331 1.00 15.62 A 73.423 56.096 CB GLN 227 ATOM 1617 C 1.00 16.35 A 73.246 12.799 57.514 227 CG GLN ATOM 1618 C 1.00 14.31 A 74.191 11.666 57.847 CD GLN 227 ATOM 1619 1.00 18.11 A 0 57.877 75.408 11.851 GLN 227 1620 0E1 ATOM 73.639 1.00 12.45 A N 10.486 58, 101 GLN 227 **ATOM** 1621 NE2 15.723 1.00 16.27 A C 73.073 56.615 227 ATOM 1622 C GLN 1.00 16.33 0 74.159 16.225 A 56.346 1623 GLN 227 **ATOM** 0 1.00 17.36 N 16.158 A 72.301 57.601 1624 N PHE 228 ATOM 1.00 16.81 A C 17.287 72.717 58.414 1625 PHE 228 ATOM CA C 1.00 14.62 A 58.327 71.686 18.412 1626 CB PHE 228 **ATOM** C 71.295 1.00 14.48 A 56.919 18.758 CG PHE 228 1627 **ATOM** Č 56.317 70.196 1.00 14.37 Α 18.141 1628 CD1 PHE 228 **ATOM** 1.00 12.73 C 72.036 19.674 A 56.183 1629 CD2 PHE 228 **ATOM** C 1.00 13.56 69.840 18.430 Α 55.007 1630 CE1 PHE 228 **ATOM** CCC 1.00 14.73 71.691 19.971 A 54.870 1631 CE2 PHE 228 **ATOM** 1.00 15.31 A 70.588 228 54.279 19.348 1632 CZPHE **ATOM** C 59.848 72.922 16.859 1.00 18.12 A 1633 PHE 228 C **ATOM** 0 60.410 72.121 16.112 1.00 17.47 Α 0 PHE 228 1634 **ATOM** N 60.413 74.027 17.335 1.00 20.00 A ASN 229 1635 N ATOM C 1.00 20.87 Α 74.435 17.042 61.779 ASN 229 1636 CA ATOM C 1.00 21.57 75.857 16.474 A 61.767 ASN 229 ATOM 1637 CB C 1.00 24.35 76.257 15.870 A 63.086 ASN 229 **ATOM** 1638 CG 0 1.00 26.00 A 75.774 16.289 OD1 ASN 229 64.141 1639 ATOM N 1.00 25.62 A 63.025 77.153 14.887 ASN 229 1640 ND2 ATOM C 62.540 18.362 1.00 21.39 A 74.421 ASN 229 1641 C ATOM 62. 232 63. 516 0 75.200 19.269 1.00 21.52 A ASN 229 1642 0 ATOM 1.00 20.96 N 18.481 A 73.530 ASP 230 ATOM 1643 N C 1.00 22.78 19.706 64.300 73.444 Α ASP **ATOM** 1644 CA 230 C 1.00 22.69 20.268 A 72.026 230 64.275 ATOM 1645 CB ASP 20.580 1.00 22.37 A 71.551 1646 CG ASP 230 62.880 **ATOM** 0 1.00 21.57 21.689 A OD1 ASP 230 62.681 71.015 1647 ATOM 0 61.993 71.705 19.713 1.00 21.82 A OD2 ASP 230 1648 ATOM Ċ 65.734 73.825 19.412 1.00 24.50 A ASP 230 1649 C **ATOM** 73. 252 1.00 24.72 0 19.979 A **ASP** 230 66.663 ATOM 1650 0 N 1.00 25.87 A 231 65.904 74.803 18.527 THR ATOM 1651 N C 75.245 18.122 1.00 26.22 A 67.228 THR 231 **ATOM** 1652 CA C 76.406 17.109 1.00 27.87 Α 231 67.149 1653 CB THR ATOM 0 1.00 28.62 A 231 66.540 75.947 15.893 0G1 THR 1654 **ATOM** C 16.813 1.00 26.63 A 231 68.545 76.947 ATOM 1655 CG2 THR C 75.688 19.280 1.00 26.77 A 68.099 231 C THR 1656 ATOM 19.375 0 1.00 27.34 69.254 75.277 A 0 231 THR 1657 ATOM N 67.550 76.519 20.163 1.00 25.50 A 232 N **ATOM** 1658 GLU C 77.020 21.285 1.00 24.52 Α 232 68.329 1659 CA **GLU** ATOM C 78.526 21.397 1.00 28.36 A 232 68.154 CB GLU 1660 **ATOM** C 68.615 79.281 20.171 1.00 34.72 A **GLU** 232 CG ATOM 1661 1.00 40.02 232 80.780 20.338 A 68.483 1662 CD **GLU ATOM** 19.363 1.00 44.21 A 0 81.509 1663 0E1 GLU 232 68.767 **ATOM** 1.00 42.26 0 81.232 21.444 A OE2 GLU 23268.100 1664 **ATOM** C 1.00 22.97 232 76.377 22.627

SUBSTITUTE SHEET (RULE 26)

68.020

GLU

1665

ATOM

C

				FIG. 4-35	(Continued)
ATOM ATOM ATOM	1666 1667 1668	O GLU N VAL CA VAL	232 233 233	68. 331 76. 942 23. 679 1. 00 20. 81 A 67. 416 75. 194 22. 596 1. 00 20. 32 A 67. 091 74. 499 23. 832 1. 00 17. 88 A 65. 853 73. 618 23. 648 1. 00 17. 88	ł.	O N C C
ATOM ATOM ATOM	1669 1670 1671	CB VAL CG1 VAL CG2 VAL	233 233 233	65.522 72.925 24.957 1.00 14.00 A 64.678 74.478 23.160 1.00 16.73	A A	C C C
ATOM ATOM	1673 1674	C VAL O VAL N PRO	233 233 234	68. 694 72. 728 23. 606 1. 00 15. 94 68. 788 73. 927 25. 504 1. 00 14. 51	4 4 4	O N C
ATOM ATOM ATOM	1675 1676 1677	CD PRO CA PRO CB PRO	234 234 234	69.914 73.162 26.040 1.00 13.93 70.031 73.677 27.473 1.00 12.63	A A A	C C C
ATOM ATOM ATOM ATOM	1678 1679 1680 1681	CG PRO C PRO O PRO N LEU	234 234 234 235	69. 643 71. 663 25. 987 1. 00 16. 20 68. 487 71. 220 26. 041 1. 00 15. 73	A A A	C O N
ATOM ATOM ATOM	1682 1683 1684	CA LEU CB LEU CG LEU	235 235 235 235	70. 602 69. 443 25. 825 1. 00 16. 91 71. 505 68. 912 24. 718 1. 00 18. 54	A A A	C C C
ATOM ATOM ATOM	1685 1686 1687	CD1 LEU CD2 LEU C LEU	235 235 235	72. 434 68. 856 22. 412 1. 00 21. 90 69. 946 68. 790 22. 768 1. 00 19. 17	A A A	C C C
ATOM ATOM ATOM	1688 1689 1690	O LEU N ILE CA ILE	235 236 236	71. 939 69. 157 27. 793 1. 00 18. 36 70. 244 67. 696 27. 472 1. 00 14. 95	A A A	O N C
ATOM ATOM ATOM	1691 1692 1693	CB ILE CG2 ILE CG1 ILE	236 236 236	68. 538 65. 433 28. 329 1. 00 9. 32 69. 806 65. 298 30. 448 1. 00 8. 74	A A A	C C C
ATOM ATOM ATOM	1694 1695 1696	CD1 ILE C ILE O ILE	236 236 236	71. 444 65. 802 28. 010 1. 00 12. 84 71. 105 65. 276 26. 942 1. 00 10. 11	A A A	C C O
ATOM ATOM ATOM	1697 1698 1699	N GLU CA GLU CB GLU	237 237 237	73. 463 64. 470 28. 128 1. 00 14. 46 74. 767 65. 128 27. 655 1. 00 13. 45	A A A	N C C
ATOM ATOM ATOM	1700 1701 1702		237 237 237	75. 845 66. 500 25. 819 1. 00 23. 46 75. 779 67. 016 24. 683 1. 00 25. 80	A A A A	C C O O
ATOM ATOM ATOM ATOM	1703 1704 1705 1706	OE2 GLU C GLU O GLU N TYR	237 237 237 238	73. 744 63. 427 29. 191 1. 00 13. 41 73. 895 63. 752 30. 363 1. 00 14. 43	A A A	C O N
ATOM ATOM ATOM	1707 1708 1709	CA TYR CB TYR CG TYR	238 238 238	74. 052 61. 093 29. 721 1. 00 14. 06 72. 810 60. 840 30. 595 1. 00 12. 42	A A A	C C C
ATOM ATOM ATOM	1710 1711 1712	CD1 TYR CE1 TYR CD2 TYR	238 238 238	71. 451 59. 139 29. 317 1. 00 16. 12 70. 292 58. 739 28. 635 1. 00 17. 09	A A A	C C C
ATOM ATOM	1713 1714	CE2 TYR CZ TYR	238 238	69. 336 60. 913 29. 020 1. 00 12. 94	A A	C C

										(Continued)
					FI	G. 4 -	36			, -
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	1715 1716 1717 1718 1719 1720 1721 1722 1723 1724 1725 1726 1727 1728 1729 1730 1731 1732 1733 1734 1735 1736 1737 1738 1739 1740 1741 1742 1743	C TO	ER 2: HE 2: YR 2:	18 74 18 74 19 75 19 75 19 75 19 76 19 76 19 76 19 76 10 76 10 76 10 76 10 76 10 76 10 76 10 76 10 77 10 76 10 77 10 77 10 77 10 77 10 77 10 77 10 77 10 77 10 77 10 77 10 77 10 77 10 77 10 77 10 77 10 77 10 77 10 77 10 77	3. 127 4. 445 4. 059 5. 220 5. 689 6. 926 7. 902 4. 661 3. 755 4. 809 3. 972 3. 003 4. 896 6. 824 1. 980 9. 859 1. 018 9. 954 5. 722 5. 129 6. 147 6. 526 6. 833 8. 065 8. 326 6. 106 7. 338	59. 257 59. 847 59. 667 58. 986 57. 779 57. 251 58. 265 56. 668 56. 587 55. 834 54. 678 54. 833 54. 037 52. 655 53. 064 51. 675 51. 878 53. 652 53. 805 52. 617 52. 167 52. 821 53. 894 52. 610 53. 678 54. 319	27. 775 28. 954 27. 798 29. 596 28. 943 29. 656 29. 766 28. 879 29. 700 27. 862 27. 679 26. 523 26. 574 27. 436 25. 858 27. 597 26. 012 26. 888 27. 330 26. 335 28. 153 27. 958 29. 329 30. 317 30. 308 31. 168 31. 218 32. 080 32. 046	1. 00 15. 96 1. 00 15. 25 1. 00 17. 74 1. 00 14. 10 1. 00 13. 87 1. 00 11. 90 1. 00 18. 76 1. 00 13. 45 1. 00 12. 12 1. 00 12. 12 1. 00 12. 12 1. 00 10. 15 1. 00 10. 15 1. 00 10. 78 1. 00 11. 95 1. 00 10. 46 1. 00 14. 83 1. 00 13. 74 1. 00 13. 74 1. 00 13. 69 1. 00 10. 88 1. 00 11. 93 1. 00 9. 47 1. 00 12. 15 1. 00 12. 15 1. 00 12. 15 1. 00 12. 15 1. 00 12. 15	A A A A A A A A A A A A A A A A A A A	(Continued) 0 C 0 N C C C C C C C C C C C C C C C
ATOM ATOM ATOM ATOM ATOM ATOM	1744 1745 1746 1747 1748 1749	C 1 0 1 N 2 CA 2	FYR 2 FYR 2 SER 2 SER 2	41 7 41 7 42 7 42 7	7. 556 5. 793 6. 686 4. 501 4. 053 4. 464	55. 408 50. 510 49. 948 50. 204 49. 180 49. 590	32. 859 26. 967 26. 322 26. 837 25. 888 24. 469	1.00 10.38 1.00 14.62 1.00 12.20 1.00 16.13 1.00 16.30	A A A A A	0 C O N C C
ATOM ATOM ATOM ATOM ATOM	1750 1751 1752 1753 1754	OG S C S O S N A CA A	SER 2 SER 2 SER 2 ASP 2 ASP 2	42 7 42 7 42 7 43 7 43 7	4. 004 4. 647 5. 219 4. 516 5. 066	48. 674 47. 816 47. 625 46. 865 45. 535	23. 496 26. 226 27. 303 25. 312 25. 548 24. 369	1.00 17.85 1.00 17.46 1.00 19.13 1.00 19.34 1.00 23.36 1.00 27.30	A A A A A	0 C O N C C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	1755 1756 1757 1758 1759 1760 1761 1762 1763	CG A OD1 A OD2 A C A N C	ASP 2 ASP 2 ASP 2 ASP 2 ASP 2 GLU 2	43 7 43 7 43 7 43 7 43 7 44 7 44 7	44. 774 73. 290 72. 549 72. 862 73. 298 74. 016 75. 016 78. 412 78. 534	44. 419 44. 246 44. 438 45. 554 46. 432 44. 559 44. 363	24. 303 24. 132 25. 126 22. 955 25. 805 25. 330 26. 567 26. 944 27. 605	1.00 21.30 1.00 33.83 1.00 36.97 1.00 37.15 1.00 23.56 1.00 22.48 1.00 24.45 1.00 23.73	A A A A A A A	C O O C O N C

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												(Cor	ntinued)
					F	Ι (G. 4	- 37				(C01	itiliueu/
ATOM	1764	CG	GLU	244	79. 9	40	42.547	27. 995	1 00	29. 35	Α	С	
ATOM	1765		GLU	244	79. 9		41. 177	28.667		29. 80	A	Č	
ATOM	1766	0E1		244	81.0		40.680	28, 958		29. 53	Ä	ŏ	
ATOM	1767	0E2		244	78. 8		40.601	28.903		29. 32	A	Ŏ	
ATOM	1768		GLU	244	79. 3		44.476	25.754	1.00	22. 28	A	C	
ATOM	1769		GLU	244	80.5		44.854	25.913		21.94	Α	0	
ATOM	1770	N	SER	245	78.8	88	44. 159	24.561	1.00	21.62	Α	N	
ATOM	1771		SER	245	79.7		44.205	23.370		19.92	Α	С	
ATOM	1772		SER	245	79.0		43.402	22. 244		19.31	A	C	
ATOM	1773		SER	245	77. 9		44.068	21.723		17. 93	A	0	
ATOM	1774	C	SER	245	80.0		45.605	22.861		19.58	A	C	
ATOM	1775		SER	245	80.8		45. 762	21.971		21.35	A	0	
ATOM	1776		LEU	246	79.3		46.628	23.397		18.69	A	N	
ATOM	1777		LEU	246	79.6		47. 983	22. 943		18.41	A	C	
ATOM	1778		LEU	246	78. 5		48. 926	23. 229		18. 20	A	C	
ATOM ATOM	1779 1780	CG CD1	LEU	$\begin{array}{c} 246 \\ 246 \end{array}$	78. 6		50.368	22. 728		17. 99 16. 83	A	C	
ATOM	1781	CD1		$240 \\ 246$	78. 7 77. 4		50. 388 51. 181	21. 214 23. 192		19. 98	A A	C	
ATOM	1782		LEU	246	80. 9		48. 463	23. 679		18. 12	A	C	
ATOM	1783		LEU	246	80. 9		48. 662	24. 895		16. 12	A	0	
ATOM	1784		GLN	247	82. 0		48. 635	22. 940		17.84	A	N	
ATOM	1785		GLN	247	83. 2		49.073	23. 532		17. 30	A	Č	
ATOM	1786		GLN	247	84. 4		49. 038	22. 480		15.11	A	Č	
ATOM	1787		GLN	247	85. 7		49. 234	23. 045		17.62	Ä	č	
ATOM	1788		GLN	247	86.8		48.770	22.090		18.47	Ä	č	
ATOM	1789	0E1		247	86.8		49.065	20.899		20.53	A	Ō	
ATOM	1790	NE2		247	87.8	32	48.049	22.611		17.76	Α	N	•
ATOM	1791		GLN	247	83. 2		50.461	24.170	1.00	17.66	Α	C	
ATOM	1792		GLN	247	83. 6		50.648	25.313		17.56	Α	0	
ATOM	1793		TYR	248	82. 7		51.436	23.430		18.50	Α	N	
ATOM	1794		TYR	248	82. 5		52. 794	23.954		19.00	Α	C	
ATOM	1795		TYR	248	83. 1		53.822	22.972		17.39	Α	С	
ATOM	1796		TYR	248	84.6		53.820	22.860		16.80	A	C	
ATOM	1797		TYR	248	85. 3		52.812	22.172		17. 20	Ą	C	
ATOM	1798	CE1		248	86. 7		52.814	22.058		17.58	A	C	
ATOM ATOM	1799 1800	CD2 CE2		248	85.4		54.838	23. 437		17.77	A	C	
ATOM	1801		TYR	248 248	86. 83		54.851	23. 333		17. 22	A	C	
ATOM	1802		TYR	248 248	87. 4′ 88. 89		53. 836	22.647		18. 42 19. 27	A	C	
ATOM	1802		TYR	248	81. 13		53. 809 53. 134	22. 595 24. 212		18.87	A	0	
ATOM	1804		TYR	248	80. 28		53. 018	23. 323		19.15	A A	C 0	
ATOM	1805		PRO	249	80. 80		53. 549	25. 440		18. 20	A	N	
ATOM	1806		PRO	249	81.6		53. 595	26.668		18. 21	A	C	
ATOM	1807		PRO	249	79. 41		53.886	25.716		18.83	A	Č	
ATOM	1808		PRO	249	79. 42		54. 222	27. 206		19.46	A	C	
ATOM	1809		PRO	249	80. 89		54. 582	27. 481		17.63	A	č	•
ATOM	1810		PRO	249	78. 93		55. 042	24.852		19.66	A	č	
ATOM	1811		PRO	249	79. 73		55. 864	24. 413		20.92	Ä	ŏ	
ATOM	1812	N I	LYS	250	77. 63		55.096	24. 599	1.00	19.01	Α	N	

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					FI	G. 4	- 39			
ATOM	1862	CB	TYR	256	65. 801	68.006	28. 077	1.00 10.57	A	C
ATOM	1863	CG	TYR	256	65.044	67.706	29. 351	1.00 10.49 1.00 9.61	A A	C ·
ATOM	1864	CD1		256	64. 949 64. 296	68. 646 68. 351	30. 378 31. 571	1.00 9.01	A	C
ATOM	1865 1866	CE1 CD2		256 256	64. 460	66. 460	29. 549	1.00 9.65	A	Č
ATOM ATOM	1867	CE2		256	63. 799	66. 156	30. 735	1.00 11.05	A	č
ATOM	1868	CZ	TYR	256	63. 722	67. 105	31.742	1.00 10.10	Α	C
ATOM	1869	OH	TYR	256	63.060	66.801	32.909	1.00 10.49	Α	0
ATOM	1870	C	TYR	256	65. 488	70.492	28.012	1.00 12.70	A	C
ATOM	1871	0	TYR	256	66. 559	70. 750	28. 553	1.00 15.49	A	0
ATOM	1872	N	PRO	257	64. 444	71.325	28.080	1.00 12.39	A	N C
ATOM	1873	CD	PRO	257	63.174	71. 254 72. 593	27. 334 28. 800	1.00 13.82 1.00 11.47	A A	C C
ATOM	1874	CA	PRO	257 257	64. 548 63. 501	73. 450	28. 106	1.00 11.41	A	č
ATOM ATOM	1875 1876	CB CG	PRO PRO	257	62. 405	72. 464	27. 866	1.00 12.87	Ä	č
ATOM	1877	C	PRO	257	64. 296	72. 489	30. 298	1.00 12.85	A	Č
ATOM	1878	ŏ	PRO	257	63. 174	72. 210	30.723	1.00 15.59	Α	0
ATOM	1879	N	LYS	258	65. 327	72.718	31.105	1.00 11.64	Α	N
ATOM	1880	CA	LYS	258	65. 155	72.671	32. 546	1.00 11.10	. A	C
ATOM	1881	CB	LYS	258	66. 501	72. 439	33. 227	1.00 12.96	A	C
ATOM	1882	CG	LYS	258	67. 034	71.012	33. 031	1.00 14.20	A	C
ATOM	1883	CD	LYS	258	68. 519	70. 906 69. 480	33. 331 33. 136	1.00 13.34 1.00 13.95	A A	C C
ATOM ATOM	1884 1885	CE NZ	LYS LYS	258 258	69. 042 68. 671	68. 536	34. 223	1.00 13.33	A	N
ATOM	1886	C	LYS	258	64. 517	73. 984	33.011	1.00 12.44	Ä	Ċ
ATOM	1887	ŏ	LYS	258	64. 368	74. 921	32. 224	1.00 11.13	A	Ö
ATOM	1888	Ň	ALA	259	64. 124	74.043	34.280	1.00 13.33	Α	N
ATOM	1889	CA	ALA	259	63.484	75. 236	34.844	1.00 14.81	Α	С
ATOM	1890	CB	ALA	259	63.368	75.097	36. 355	1.00 16.40	A	C
ATOM	1891	C	ALA	259	64. 167	76. 555	34.508	1.00 15.14	A	C
ATOM	1892	0	ALA	259	65. 317	76. 787	34. 881	1.00 17.32	A	0 N
ATOM	1893	N CA	GLY GLY	260	63. 448 63. 984	77. 419 78. 720	33. 802 33. 444	1.00 16.82 1.00 15.59	A A	N C
ATOM ATOM	1894 1895	CA	GLY	260 260	64. 870	78. 749	32. 217	1.00 15.33	A	Č
ATOM	1896	Ö	GLY	260	65. 379	79. 812	31.852	1.00 17.65	Ä	ŏ
ATOM	1897	N	ALA	261	65.072	77.600	31.577	1.00 13.77	A	Ň
ATOM	1898	CA	ALA	261	65.906	77.554	30.379	1.00 11.19	Α	С
ATOM	1899	CB	ALA	261	66.524	76.182	30.224	1.00 10.21	Α	C
ATOM	1900	C	ALA	261	65.093	77.911	29. 137	1.00 10.04	A	C
ATOM	1901	0	ALA	261	63.896	78. 160	29. 212	1.00 8.71	A	0
ATOM	1902	N	VAL	262	65. 747	77. 947	27. 987	1.00 11.73	A	N C
ATOM	1903	CA	VAL	262	65.050	78. 284	26. 761	1.00 12.13	A A	C C C
ATOM	1904 1905	CB CG1	VAL VAL	262 262	66. 035 65. 257	78. 529 78. 796	25. 594 24. 299	1.00 11.50 1.00 8.31	A	C .
ATOM ATOM	1905		VAL	262	66. 939	79. 732	25. 920	1.00 5.79	A	č
ATOM	1907	C	VAL	262	64.092	77. 167	26. 389	1.00 13.92	A	č
ATOM	1908	Ŏ	VAL	262	64. 471	76.001	26. 341	1.00 16.73	Α	0
ATOM	1909	N	ASN	263	62.844	77. 536	26. 139	1.00 13.49	A	N
ATOM	1910	CA	ASN	263	61.816	76. 585	25. 773	1.00 13.67	A	C

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										(Cont	tinued)
					FΙ	G. 4	- 40				
ATOM	1911	СВ	ASN	263	60. 470	77. 038	26.336	1.00 14.53	A	C	
ATOM	1912		ASN	263	60.222	76.545	27.746	1.00 17.27	Α	С	
ATOM	1913	0D1		263	59.342	77.058	28.444	1.00 18.62	Α	0	
ATOM	1914	ND2		263	60.977	75.534	28. 169	1.00 16.78	A	Ŋ	
ATOM	1915	C	ASN	263	61.715	76.500	24. 265	1.00 14.45	A	C	
ATOM	1916		ASN	263	62.170	77. 395	23. 561	1.00 16.33	A	0	
ATOM	1917		PR0	264		75.418	23. 743	1.00 14.86	Ą	N	
ATOM	1918		PR0	264	60. 513	74. 254	24. 412	1.00 15.86	A	C	
ATOM	1919		PR0	264	60. 986	75. 301	22. 294	1.00 15.41	A	C	
ATOM	1920		PR0	264	60. 591	73.844	22. 106	1.00 14.97	A	C	
ATOM	1921		PRO	264	59. 721	73.607	23. 287 21. 882	1.00 14.81 1.00 15.66	A A	Č	
ATOM	1922		PRO	264	59. 867 58. 954	76. 238 76. 496	22. 663	1.00 13.00	A	Õ	
ATOM	1923		PRO	$\begin{array}{c} 264 \\ 265 \end{array}$	59. 942	76. 767	20. 673	1.00 17.42	A	N	
ATOM	1924	N CA	THR THR	265 265	58. 895	77.648	20. 199	1.00 14.67	Ä	Ĉ	
ATOM ATOM	1925 1926	CB	THR	265	59. 458		19. 341	1.00 15.37	A	Č	
ATOM	1927	OG1		265	60. 162	78. 228	18. 223	1.00 15.98	A	0	
ATOM	1928	CG2		265	60. 402	79.633	20. 159	1.00 12.01	Α	С	
ATOM	1929	C	THR	265	58.024		19.360	1.00 15.62	Α	С	
MOTA	1930	Ō	THR	265	58. 465		18.932	1.00 18.75	Α	0	
ATOM	1931	N	VAL	266	56. 794	77.170	19. 113	1.00 15.56	Α	N	
ATOM	1932	CA	VAL	266	55.872	76.352	18.347	1.00 12.79	A	C	
ATOM	1933	CB	VAL	266	54.856	75.692	19. 274	1.00 12.90	A	C	
ATOM	1934	CG1		266	54. 193		20. 130	1.00 12.06	A	C	
ATOM	1935	CG2		266	53. 821	74. 920	18. 466	1.00 10.69	A	C	
ATOM	1936	C	VAL	266	55. 115		17. 350	1.00 12.88	A	0	
ATOM	1937	0	VAL	266	54.995		17. 511 16. 327	1.00 12.12 1.00 13.52	A A	N	
ATOM	1938	N	LYS LYS	$\frac{267}{267}$	54. 601 53. 817		15. 262	1.00 13.02	A	Č	
ATOM ATOM	1939 1940	CA CB	LYS	267	54. 692		14. 050	1.00 13.64	A	č	
ATOM	1941	CG	LYS	267	55. 642		14. 165	1.00 13.17	A	Č	
ATOM	1942	CD	LYS	267	56. 348		12.833	1.00 11.33	A	C	
ATOM	1943	CE	LYS	267	57. 313		12.788	1.00 11.66	Α	С	
ATOM	1944	NZ	LYS	267	58.007		11.459	1.00 12.98	Α	N	
ATOM	1945	C	LYS	267	52.713		14.851	1.00 14.81	A	C	
ATOM	1946	0	LYS	267	52. 885	74.916	14. 930	1.00 14.91	A	0	
ATOM	1947	N	PHE	268				1.00 15.02	A		
ATOM	1948	CA	PHE	268	50. 471		13. 975	1.00 14.84	A	C	
ATOM	1949	CB	PHE	268	49. 249		14. 842	1.00 13.98	A	C	
ATOM	1950	CG	PHE	268	48. 237		14.846	1.00 15.65	A	C	
ATOM	1951		PHE	268	48. 467		15. 562 14. 115	1.00 15.51 1.00 18.05	A A	C	
ATOM	1952		PHE	268	47.056		15. 551	1.00 15.03	A	Č	
ATOM	1953 1954		PHE PHE	268 268	47. 537 46. 120		14. 101	1.00 13.17	A	Č	
ATOM ATOM	1954	CZ	PHE	268	46. 366		14. 821	1.00 14.54	A	č	
ATOM	1956	C	PHE	268	50. 117		12. 497	1.00 14.63	Ä	č	
ATOM	1957	ŏ	PHE	268	50. 143		11.981	1.00 16.53	Ä	Ö	
ATOM	1958	Ň	PHE	269	49.767		11.829	1.00 13.37	Α	N	
ATOM	1959	CA	PHE	269	49.417		10.413	1.00 12.73	Α	C	

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(Continued) FIG. 4-41 **ATOM** 1960 CB PHE 269 50.597 74.510 9.547 1.00 12.68 C 1961 ATOM 75. 229 CG PHE 269 51.875 9.809 1.00 10.71 C C C52.190 ATOM 1962 CD1 PHE 269 76.387 9.112 1.00 11.11 A ATOM 1963 CD2 PHE 269 52.758 74.759 10.770 1.00 11.04 A **ATOM** 1964 CE1 PHE 53.374 77.070 Ċ 269 9.371 1.00 12.54 **ATOM** 1965 CE2 PHE 269 53.940 75.430 11.039 Č 1.00 13.96 Α 54. 252 48. 270 **ATOM** 1966 CZPHE 76.591 269 10.339 1.00 13.89 C A ATOM 1967 PHE 74.032 C 269 10.117 1.00 12.37 C ATOM 1968 0 47.937 73.157 PHE 269 10.910 1.00 14.50 0 47.699 **ATOM** 1969 N 74.193 VAL 270 8.938 1.00 13.63 N ATOM 1970 73.334 CA VAL 270 46.626 8.485 1.00 15.44 C ATOM 1971 CB VAL 270 45.228 73.903 8.815 1.00 14.59 C ATOM 1972 270 44.153 CG1 VAL 72.900 8.383 1.00 12.94 Α C 1973 **ATOM** CG2 VAL 270 45.110 74.183 10.304 1.00 15.69 A C ATOM 1974 46. 730 C 270 VAL 73.198 6.975 1.00 16.91 A C ATOM 1975 0 VAL 270 46.875 74.188 6.258 1.00 17.51 A 0 **ATOM** 1976 N VAL 271 46.681 71.966 6.494 1.00 17.37 A N 1977 46.726 **ATOM** CA VAL 271 71.746 5.067 1.00 16.54 A C **ATOM** 1978 CB VAL 271 47.928 70.879 4.646 1.00 19.07 A C ATOM 1979 CG1 VAL 271 47.911 69.548 5.400 1.00 20.07 C A **ATOM** 1980 CG2 47.878 VAL 271 70.635 1.00 18.62 3.131 C A ATOM 1981 45. 456 C VAL 271 71.041 4.641 1.00 15.09 Α C 1982 1983 ATOM 0 VAL 271 44.912 70.226 5.383 1.00 13.46 A 0 ATOM N ASN 272 44.988 71.394 3.449 1.00 15.17 A N ATOM 1984 CA ASN 272 43.812 70.802 2.832 1.00 14.94 A C ATOM 1985 43. 231 CB ASN 272 71.767 1.797 1.00 13.83 A C 1986 **ATOM** CG ASN 42.010 272 71.205 1.093 1.00 14.46 A C **ATOM** 1987 OD1 ASN 272 41.822 69.989 1.007 1.00 16.67 A 0 41.175 ATOM 1988 ND2 ASN 272 72.090 0.581 1.00 15.74 A N ATOM ATOM 1989 272 C ASN 44.310 1.00 15.70 69.542 2.110 C 1990 0 **ASN** 272 44.755 69.617 0.967 1.00 16.88 A 0 **ATOM** 1991 68.390 N 273 THR 44. 241 2.758 1.00 15.93 A N **ATOM** 1992 CA 273 THR 44.717 67.169 2.124 1.00 18.97 A C 1993 ATOM THR 273 CB 44.570 65.936 3.052 1.00 19.44 C A ATOM 1994 0G1 273 43. 201 THR 65.794 3.471 1.00 19.69 0 A ATOM 1995 CG2 273 45.481 THR 66.083 4.266 1.00 19.20 C A **ATOM** 1996 C 273 44.009 THR 66.870 0.813 1.00 19.92 A C ATOM 1997 0 THR 273 -0.028 44.550 66.154 1.00 21.20 0 A ATOM 1998 N 42. 811 42. 032 274 ASP 67.424 0.634 1.00 20.50 N A 1999 **ATOM** CA **ASP** 274 67.193 -0.584 1.00 20.30 C A ATOM 2000 CB **ASP** 274 40.578 67.629 -0.390 1.00 21.02 $_{\rm C}^{\rm C}$ A ATOM 2001 CG 274 39.705 **ASP** 66.529 0.178 1.00 23.48 A **ATOM** 38. 543 2002 0D1 ASP 274 66.823 0.527 1.00 26.38 0 A **ATOM** 2003 **OD2** ASP 274 40.168 65.375 0.275 1.00 23.88 0 Α ATOM 2004 C **ASP** 274 67.870 42.573 1.00 19.89 Č -1.832A **ATOM** 2005 0 **ASP** 274 42.131 67.556 -2.9321.00 22.08 0 A ATOM 2006 N SER 275 43.508 68.802 -1.6761.00 18.13 N A

> 70.969 SUBSTITUTE SHEET (RULE 26)

69.490

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ATOM

ATOM

2007

2008

CA

CB

SER

SER

275

275

					FΙ	G. 4	- 42			(Continued)
ATOM	2009	0G	SER	275	45. 197	71.121	-1.444	1.00 24.82	A	0
ATOM	2010	C	SER	275	45. 397	68.885	-3. 314	1.00 19.53	Α	С
ATOM	2011	0	SER	275	45.883	69.226	-4. 394	1.00 19.59	Α	0
ATOM	2012	N	LEU	276	45. 971	67.986	-2.516	1.00 19.83	Α	N
ATOM	2013	CA	LEU	276	47. 241	67. 348	-2.846	1.00 20.72	Α	C
ATOM	2014	CB	LEU	276	47. 545	66. 226	-1.849	1.00 19.96	A	C
ATOM	2015	CG	LEU	276	47. 725	66.641	-0.392	1.00 20.47	A	C
ATOM	2016		LEU	276	47. 991	65. 410	0.456	1.00 21.68	A	C
ATOM	2017		LEU	276	48. 875	67. 622	-0.277	1.00 18.56	A	C
ATOM	2018	C	LEU	276	47. 360	66. 790	-4. 263	1.00 22.34	A	C
ATOM	2019	0	LEU	276	48. 290	67. 137	-4. 994	1.00 24.63	A	0 N
ATOM	2020	N	SER SER	277 277	46. 434	65. 925	-4.656	1.00 22.80 1.00 23.82	A	N C
ATOM ATOM	2021 2022	CA CB	SER	277	46. 501 45. 456	65. 325 64. 219	-5. 983 -6. 121	1.00 23.62	A	C C
ATOM	2023	OG	SER	277	44. 148	64. 756	-6.044	1.00 22.33	A A	0
ATOM	2023	C	SER	277	46. 305	66. 341	-7.097	1.00 24.47	A	C
ATOM	2025	Ö	SER	277	46. 699	66.104	-8. 231	1.00 26.86	A	ő
ATOM	2026	N	SER	278	45. 698	67. 472	-6.768	1.00 25.44	A	N
ATOM	2027	ĈA	SER	278	45. 431	68. 522		1.00 26.20	Ä	Ċ
ATOM	2028	CB	SER	278	44. 051	69. 121	-7.471	1.00 25.70	Ä	č
ATOM	2029	0G	SER	278	43. 831	70. 266	-8. 266	1.00 30.53	A	Ö
ATOM	2030	C	SER	278	46.495	69.630	-7.739	1.00 25.70	Ā	Ċ
ATOM	2031	0	SER	278	46.603	70.414	-8.683	1.00 23.48	Α	0
ATOM	2032	N	VAL	279	47. 277	69.692	-6.672	1.00 26.01	Α	N
ATOM	2033	CA	VAL	279	48. 327	70.696	-6.565	1.00 28.42	Α	C
ATOM	2034	CB	VAL	279	48.073	71.634	-5.350	1.00 29.96	Α	C
ATOM	2035		VAL	279	49. 372	72. 211	-4.834	1.00 32.19	A	C
ATOM	2036		VAL	279	47. 148	72. 768	-5. 776	1.00 29.00	A	C
ATOM	2037	C	VAL	279	49.704	70.043	-6.470	1.00 28.21	A	C
ATOM	2038	0	VAL	279	49. 834	68. 872	-6.088	1.00 29.00	A	0
ATOM	2039	N	THR	280	50. 728	70.801	-6. 848	1.00 26.67	A	N
ATOM	2040 2041	CA CB	THR THR	280	52. 092	70.306	-6.832	1.00 26.53	A	C
ATOM ATOM	2041		THR	280 280	53. 023 52. 533	71. 217 71. 331	-7. 645 -8. 986	1.00 27.22 1.00 29.98	A	C
ATOM	2042		THR	280	54. 422	70.645	-7. 674	1.00 29.98	A A	0 C
ATOM	2044	C	THR	280	52. 618	70. 254	-5. 418	1.00 26.01	A	C
ATOM	2045		THR	280	53. 184			1.00 27.33	A	Ö
ATOM	2046	Ň	ASN	281	52. 402	71.341	-4. 696	1.00 25.17	Ä	N
ATOM	2047	CA	ASN	281	52. 876	71. 474	-3. 334	1.00 23.78	Ä	Ċ
ATOM	2048	CB	ASN	281	54. 190	72. 250	-3. 388	1.00 22.28	Ä	č
ATOM	2049	CG	ASN	281	54.925	72. 287	-2.071	1.00 22.87	A	Č
ATOM	2050	OD1	ASN	281	54.603	71.576	-1.116	1.00 20.83	A	0
ATOM	2051		ASN	281	55.948	73. 136	-2.056	1.00 22.18	Α	N
ATOM	2052	C	ASN	281	51.818	72. 211	-2.506	1.00 23.12	Α	С
ATOM	2053	0	ASN	281	51.876	73. 431	-2.362	1.00 22.47	Α	0
ATOM	2054	N	ALA	282	50. 849	71.460	-1.982	1.00 23.33	A	Ŋ
ATOM	2055	CA	ALA	282	49. 763	72.018	-1.166	1.00 23.40	A	Ç
ATOM	2056	CB	ALA	282	48. 952	70. 895	-0.547	1.00 23.19	A	C
ATOM	2057	С	ALA	282	50. 320	72. 912	-0.071	1.00 24.45	A	С

					4.0		(Continued)						
F I G. 4 - 43													
ATOM ATOM ATOM	2058 2059 2060	O AL N TH CA TH	R 283	51. 180 72. 487 49. 817 74. 140 50. 326 75. 074	0.694 1.00 25.49 0.024 1.00 24.70 1.021 1.00 25.33	A A A	O N C						
ATOM ATOM	2061 2062	CB TH	R 283	50. 209 76. 540 48. 834 76. 874	0.539 1.00 27.36 0.353 1.00 29.84	A A	C 0						
ATOM	2063	CG2 TH	R 283		-0.785 1.00 30.06 2.406 1.00 24.49	A A	C C						
ATOM ATOM	2064 2065	0 TH	R 283	48. 487 74. 960	2.578 1.00 24.13	A A	0 N						
ATOM ATOM	2066 2067	N SE CA SE	R 284	50. 593 74. 941 50. 200 74. 872	4.791 1.00 19.88	Α	C						
ATOM ATOM	2068 2069	CB SE	R 284	51. 317 74. 249 51. 413 72. 868	5. 624 1. 00 15. 88 5. 350 1. 00 14. 23	A A	C 0						
ATOM ATOM	2070 2071	C SE	R 284	49. 906 76. 275 50. 774 77. 148	5. 288 1. 00 19. 24 5. 253 1. 00 18. 08	A A	C 0						
ATOM ATOM	$\begin{array}{c} 2072 \\ 2073 \end{array}$	N IL CA IL	E 285	48. 674 76. 478 48. 249 77. 771	5. 745 1. 00 17. 36 6. 242 1. 00 16. 16	A A	N C						
ATOM ATOM	$2074 \\ 2075$	CB II CG2 II		46. 754 78. 003 46. 384 79. 446	5.977 1.00 16.93 6.324 1.00 14.55	A A	C C						
ATOM ATOM	2076 2077	CG1 II CD1 II		46. 434 77. 691 47. 230 78. 526	4.513 1.00 14.89 3.528 1.00 15.03	A A	C C						
ATOM ATOM	2078 2079	C II		48. 496 77. 848 48. 116 76. 963	7. 733 1. 00 16. 46 8. 489 1. 00 18. 69	A A	C 0						
ATOM ATOM	2080 2081	N GI CA GI	N 286	49. 130 78. 923 49. 428 79. 088	8.159 1.00 16.66 9.563 1.00 16.43	A A	N C						
ATOM ATOM	2082 2083	CB GI	LN 286	50. 778 79. 776 51. 184 80. 070	9.717 1.00 16.31 11.135 1.00 17.85	A A	C C						
ATOM ATOM	2084 2085	CD GI OE1 GI	LN 286	52.552 80.713 53.072 81.005	11.196 1.00 21.44 12.277 1.00 24.09	A A	C 0						
ATOM ATOM	2086 2087	NE2 GI	LN 286	53. 149 80. 939 48. 360 79. 885	10.028 1.00 19.13 10.289 1.00 16.82	A A	N C						
ATOM ATOM	2088 2089	0 GI		47. 794 80. 844 48. 070 79. 453	9.754 1.00 17.23 11.507 1.00 15.99	A A	O N						
ATOM ATOM	2090 2091	CA II	LE 287 LE 287	47. 116 80. 137 46. 036 79. 182	12.355 1.00 15.11 12.894 1.00 14.14	A A	Č C						
ATOM ATOM ATOM	2091 2092 2093	CG2 II	LE 287	45. 147 79. 916 45. 206 78. 621	13. 875 1. 00 14. 36 11. 742 1. 00 13. 29	A A	C C						
ATOM	2094	CD1 II		44. 111 77. 675 47. 991 80. 625	12. 202 1. 00 14. 31 13. 506 1. 00 15. 35	A A	C C						
ATOM ATOM	2095 2096	0 II	LE 287 HR 288	48. 349 79, 860 48. 367 81. 894	14. 401 1. 00 14. 39 13. 452 1. 00 15. 01	A A	O N						
ATOM ATOM	2097 2098	CA TI	HR 288 HR 288	49. 215 82. 465 49. 688 83. 874	14. 482 1. 00 16. 71 14. 093 1. 00 17. 36	A A	C C						
ATOM ATOM	2099 2100	OG1 TI	HR 288	48. 548 84. 679	13.779 1.00 21.17 12.881 1.00 17.64	A A	Ö C						
ATOM ATOM	2101 2102	C TI	HR 288 HR 288	48.510 82.553	15. 818 1. 00 16. 02 15. 888 1. 00 16. 28	A A	Č O						
ATOM ATOM	2103 2104	N A	HR 288 LA 289	47. 287 82. 668 49. 301 82. 488	16.881 1.00 16.31	A A	N C						
ATOM ATOM	2105 2106		LA 289 LA 289	48. 787 82. 582 49. 887 82. 262	18. 232 1. 00 16. 67 19. 207 1. 00 18. 89	A	C						

ATOM 2108 O ALA 289 48.280 84.001 18.467 1.00 18.05 A C ATOM 2109 N PRO 290 47.436 84.193 19.487 1.00 18.60 A N ATOM 2110 CD PRO 290 46.851 83.189 20.388 1.00 19.12 A O ATOM 2110 CD PRO 290 46.851 83.189 20.388 1.00 18.37 A C C ATOM 2111 CA PRO 290 46.906 85.526 19.783 1.00 19.04 A C ATOM 2112 CB PRO 290 45.916 85.234 20.7777 1.00 17.58 A C C ATOM 2113 CG PRO 290 45.906 85.526 19.783 1.00 19.04 A C ATOM 2114 C PRO 290 44.860 84.005 21.499 1.00 19.78 A C C ATOM 2115 CD PRO 290 44.860 84.005 21.499 1.00 19.78 A C C ATOM 2115 C PRO 290 44.866 85.955 21.492 1.00 19.78 A C C ATOM 2116 N ALA 291 47.878 87.735 20.054 1.00 19.85 A N ATOM 2116 N ALA 291 47.878 87.735 20.054 1.00 19.85 A N ATOM 2116 N ALA 291 48.829 88.728 20.543 1.00 19.27 A C ATOM 2119 C ALA 291 48.829 88.728 20.441 1.00 19.85 A N ATOM 2119 C ALA 291 48.829 88.728 20.441 1.00 19.66 A C ATOM 2120 O ALA 291 50.238 88.791 22.489 1.00 21.96 A C ATOM 2121 N SER 292 48.774 88.305 21.322 20.213 1.00 17.30 A C C ATOM 2120 N ALA 291 48.00 88.30 90.132 20.213 1.00 17.30 A C C ATOM 2120 N ALA 291 48.00 88.30 90.132 20.213 1.00 17.30 A C C ATOM 2120 N ALA 291 48.00 88.30 90.132 20.213 1.00 17.30 A C C ATOM 2120 N ALA 291 48.00 88.30 90.328 20.213 1.00 17.30 A C C ATOM 2120 N ALA 291 49.101 88.610 22.441 1.00 19.66 A C ATOM 2120 N ALA 291 49.101 88.610 22.441 1.00 19.00 A C C ATOM 2125 C SER 292 48.774 88.305 22.825 1.00 19.16 A N ATOM 2126 N ALA 291 49.101 88.610 22.441 1.00 19.90 A C C ATOM 2125 C SER 292 49.48 8.705 88.83 24.971 1.00 21.90 A C C ATOM 2125 C SER 292 49.48 8.705 86.839 24.487 1.00 19.90 A C C ATOM 2125 C SER 292 49.48 87.05 86.839 24.487 1.00 19.90 A C C ATOM 2125 C SER 292 49.868 86.948 25.760 1.00 21.86 A O A C ATOM 2127 N MET 293 49.566 86.948 25.760 1.00 21.86 A O A C ATOM 2128 C MET 293 49.586 86.214 23.818 1.00 18.39 A C C ATOM 2131 SD MET 293 49.565 86.291 2.388 1.00 20.24 A C C ATOM 2131 SD MET 293 49.565 86.291 2.388 1.00 20.24 A C C ATOM 2144 C A LEU 294 52.488 87.08 88.293 26.296 1.00 15.89 A C C ATOM 2144 C A LEU 294 52.488 87.588 22.9					FIG 4-44	(Continued)
ATOM 2147 CG1 ILE 295 52.906 89.034 25.998 1.00 25.57 A C ATOM 2148 CD1 ILE 295 52.157 89.761 27.085 1.00 26.45 A C ATOM 2149 C ILE 295 55.271 88.426 24.565 1.00 21.97 A C ATOM 2150 O ILE 295 56.218 89.064 25.006 1.00 23.91 A O ATOM 2151 N GLY 296 55.154 87.119 24.749 1.00 20.65 A N ATOM 2152 CA GLY 296 56.174 86.401 25.482 1.00 18.90 A C ATOM 2153 C GLY 296 56.165 84.922 25.167 1.00 18.45 A C ATOM 2154 O GLY 296 55.527 84.503 24.202 1.00 18.61 A O	ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2108 2109 2110 2111 2112 2113 2114 2115 2116 2117 2118 2119 2120 2121 2122 2123 2124 2125 2126 2127 2128 2129 2130 2131 2132 2133 2134 2135 2136 2137 2138 2136 2137 2138 2142 2142 2143 2144 2143 2144 2145	O ALA N PRO CD PRO CCA ALA CCB ALA CCB ALA CCB SER CC O SER CC SER CC O MET CCB MET CCB LEU CCC LEU CCC CCC CCC O N CCCC CCC CCCC CCCC CCCC CCCC CCCC CCCC CCCCC CCCC CCCCC CCCCC CCCCCC	289 290 290 290 290 291 291 291 291 291 292 292 292 293 293 293 293 293 294 294 294 294 294 294 295 295 295 295 295 295 295 296	48. 629 84. 927 17. 733 1. 00 19. 12 47. 436 84. 193 19. 487 1. 00 18. 60 46. 851 83. 189 20. 388 1. 00 18. 37 46. 906 85. 526 19. 783 1. 00 19. 04 45. 791 85. 234 20. 777 1. 00 17. 58 46. 306 84. 055 21. 499 1. 00 19. 78 47. 976 86. 447 20. 369 1. 00 20. 45 48. 866 85. 995 21. 092 1. 00 19. 85 48. 829 88. 728 20. 543 1. 00 19. 85 48. 829 88. 728 20. 543 1. 00 19. 27 48. 330 90. 132 20. 213 1. 00 17. 30 49. 101 88. 610 22. 041 1. 00 19. 66 50. 238 88. 791 22. 489 1. 00 21. 52 48. 074 88. 305 22. 825 1. 00 19. 97 46. 936 87. 983 24. 971 1. 00 19. 97 46. 936 86. 839 24.	A C C C C C C C C C C C C C C C C C C C
ATOM 2150 0 ILE 295 56. 218 89. 064 25. 006 1. 00 23. 91 A O ATOM 2151 N GLY 296 55. 154 87. 119 24. 749 1. 00 20. 65 A N ATOM 2152 CA GLY 296 56. 174 86. 401 25. 482 1. 00 18. 90 A C ATOM 2153 C GLY 296 56. 165 84. 922 25. 167 1. 00 18. 45 A C ATOM 2154 0 GLY 296 55. 527 84. 503 24. 202 1. 00 18. 61 A O	ATOM ATOM ATOM ATOM ATOM	2145 2146 2147 2148	CB ILE CG2 ILE CG1 ILE CD1 ILE	295 295 295 295	53. 323 89. 938 24. 835 1. 00 24. 92 52. 084 90. 536 24. 196 1. 00 25. 08 52. 906 89. 034 25. 998 1. 00 25. 57 52. 157 89. 761 27. 085 1. 00 26. 45	A C A C A C A C
ATOM THE ALL ASD TOTAL SERVICE	ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2148 2149 2150 2151 2152 2153 2154	CD1 ILE C ILE O ILE N GLY CA GLY C GLY O GLY	295 295 295 296 296 296 296	52. 157 89. 761 27. 085 1. 00 26. 45 55. 271 88. 426 24. 565 1. 00 21. 97 56. 218 89. 064 25. 006 1. 00 23. 91 55. 154 87. 119 24. 749 1. 00 20. 65 56. 174 86. 401 25. 482 1. 00 18. 90 56. 165 84. 922 25. 167 1. 00 18. 45 55. 527 84. 503 24. 202 1. 00 18. 61	A C A C A O A N A C A C A O

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	٠			FIG. 4-45	(Continued)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2156 2157 2158 2159 2160 2161 2162 2163 2164 2165	CA ASP CB ASP CG ASP OD1 ASP OD2 ASP C ASP O ASP N HIS CA HIS CB HIS	297 297 297 297 297 297 297 298 298 298	56. 918 82. 694 25. 751 1. 00 16. 95 A 57. 960 82. 032 26. 650 1. 00 18. 00 A 59. 366 82. 378 26. 253 1. 00 18. 62 A 59. 553 82. 882 25. 128 1. 00 18. 23 A 60. 284 82. 134 27. 063 1. 00 21. 29 A 55. 553 82. 096 26. 041 1. 00 16. 02 A 54. 847 82. 537 26. 942 1. 00 16. 36 A 55. 190 81. 079 25. 279 1. 00 14. 79 A 53. 901 80. 449 25. 460 1. 00 16. 82 A 52. 846 81. 207 24. 661 1. 00 14. 81 A	A C A C A O A C A C A O A N
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2166 2167 2168 2169 2170 2171 2172 2173 2174	CG HIS CD2 HIS ND1 HIS CE1 HIS NE2 HIS C HIS O HIS N TYR CA TYR	298 298 298 298 298 298 298 298 299	52. 840 81. 207 24. 001 1. 00 14. 81 7 53. 245 81. 448 23. 241 1. 00 15. 31 7 52. 921 80. 793 22. 099 1. 00 14. 85 7 54. 127 82. 442 22. 876 1. 00 13. 01 7 54. 327 82. 392 21. 572 1. 00 14. 39 7 53. 608 81. 400 21. 076 1. 00 14. 38 7 53. 956 79. 008 24. 979 1. 00 17. 54 7 55. 008 78. 519 24. 560 1. 00 15. 53 7 52. 802 78. 348 25. 031 1. 00 17. 25 7 52. 675 76. 963 24. 609 1. 00 16. 58 7	A C A C A N A C A N A C A O A N
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2175 2176 2177 2178 2179 2180 2181 2182 2183	CB TYR CG TYR CD1 TYR CE1 TYR CD2 TYR CE2 TYR CZ TYR OH TYR C TYR	299 299 299 299 299 299 299 299	52. 666 76. 029 25. 816 1. 00 15. 77 A 53. 811 76. 176 26. 790 1. 00 17. 03 A 55. 095 75. 762 26. 456 1. 00 14. 29 A 56. 119 75. 807 27. 380 1. 00 15. 79 A 53. 586 76. 653 28. 081 1. 00 15. 17 A 54. 600 76. 700 29. 009 1. 00 15. 67 A 55. 865 76. 270 28. 656 1. 00 15. 90 A 56. 863 76. 261 29. 595 1. 00 16. 73 A 51. 351 76. 741 23. 893 1. 00 17. 76 A	C C C C C C C C C C C C C C C C C C C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2184 2185 2186 2187 2188 2189 2190	O TYR N LEU CA LEU CB LEU CG LEU CD1 LEU CD2 LEU C LEU O LEU	299 300 300 300 300 300 300 300 300	50. 349 77. 411 24. 178 1. 00 16. 87 A 51. 355 75. 799 22. 959 1. 00 16. 20 A 50. 130 75. 413 22. 292 1. 00 16. 36 A 50. 413 74. 923 20. 878 1. 00 16. 40 A 49. 232 74. 296 20. 139 1. 00 14. 78 A 48. 131 75. 322 19. 972 1. 00 16. 55 A 49. 692 73. 789 18. 785 1. 00 15. 08 A 49. 777 74. 243 23. 205 1. 00 17. 58 A 50. 568 73. 312 23. 335 1. 00 17. 21 A	0 1 N 1 C 1 C 1 C 1 C 1 C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2193 2194 2195 2196 2197 2198 2199 2200 2201 2202	N CYS CA CYS CB CYS SG CYS C CYS O CYS N ASP CA ASP CB ASP CG ASP	301 301 301 301 301 302 302 302 302	48. 629 74. 290 23. 873 1. 00 19. 46 A 48. 288 73. 202 24. 782 1. 00 22. 20 A 48. 208 73. 722 26. 220 1. 00 22. 63 A 46. 943 74. 962 26. 503 1. 00 26. 56 A 47. 032 72. 399 24. 468 1. 00 23. 29 A 46. 690 71. 481 25. 210 1. 00 25. 66 A 46. 341 72. 731 23. 386 1. 00 23. 55 A 45. 148 71. 976 23. 015 1. 00 24. 19 A 43. 999 72. 223 23. 991 1. 00 26. 49 A 42. 789 71. 355 23. 680 1. 00 28. 68 A	N C C C C C
ATOM ATOM	2203 2204	OD1 ASP OD2 ASP	302 302	42. 795 70. 170 24. 066 1. 00 30. 65 A 41. 841 71. 844 23. 029 1. 00 30. 37 A	. 0

(Continued)

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					FIC	G. 4-	46			(0020
ATOM	2205	С	ASP	302	44.658	72. 292	21.610	1.00 23.22	A	C
ATOM	2206		ASP	302	44.523	73. 455	21. 226	1.00 24.26	Ą	0
ATOM	2207		VAL	303	44.385	71. 237	20.857	1.00 21.65	A	N
ATOM	2208	CA	VAL	303	43.902	71.349	19. 493	1.00 20.79	A	C
ATOM	2209		VAL	303	44.926	70. 803	18. 480	1.00 21.88	A	C
ATOM	2210		VAL	303	44. 420	71.028	17.051	1.00 20.34	A	C C
ATOM	2211		VAL	303	46. 273	71.465	18. 702 19. 417	1.00 20.12 1.00 20.38	A A	C
ATOM	2212	C	VAL	303	42.657	70. 494 69. 306	19. 417	1.00 20.38	A	0
ATOM	2213	0	VAL	303	42.687 41.562	71.102	18. 982	1.00 13.46	A	N
ATOM	2214	N	THR THR	304 304	40.302	70. 394	18. 882	1.00 19.30	Ä	ĉ
ATOM	2215	CA CB	THR	304 304	39. 494	70.546	20. 191	1.00 19.73	Ä	Č
ATOM ATOM	2216 2217	OG1	THR	304	40. 256	70.024	21. 287	1.00 20.19	A	0
ATOM	2218	CG2	THR	304	38. 168	69.812	20.090	1.00 17.51	Α	C
ATOM	2219	C	THR	304	39. 467	70.930	17.733	1.00 18.56	Α	С
ATOM	2220	ŏ	THR	304	39. 185	72.127	17.674	1.00 19.32	Α	0
ATOM	2221	Ň	TRP	305	39.082	70.042	16.819	1.00 18.08	A	N
ATOM	2222	CA	TRP	305	38. 243	70.422	15.681	1.00 16.88	A	C
ATOM	2223	CB	TRP	305	38. 332	69.394	14. 546	1.00 13.92	A	C
ATOM	2224	CG	TRP	305	39. 581	69.464	13. 745	1.00 13.82	A	C
ATOM	2225	-	TRP	305	39. 815	70. 296	12.606	1.00 13.04	A	C C
ATOM	2226	CE2	TRP	305	41. 143	70.068	12.189	1.00 13.12 1.00 13.55	A A	C
ATOM	2227		TRP	305	39.031	71. 216 68. 781	11. 899 13. 967	1.00 13.55	A	Č
ATOM	2228	CD1	TRP TRP	305 305	40. 745 41. 688	69. 138	13. 036	1.00 11.41	A	N
ATOM	2229 2230	NE1	TRP	305 305	41.704	70. 729	11.094	1.00 12.03	Ä	Ċ
ATOM ATOM	2230 2231	CZ3	TRP	305 305	39. 591	71.873	10. 809	1.00 14.16	Ä	č
ATOM	2232	CH2	TRP	305	40. 914	71.625	10.419	1.00 13.92	A	C
ATOM	2233	C	TRP	305	36. 803	70.477	16.155	1.00 16.35	Α	С
ATOM	2234	ŏ	TRP	305	36. 368	69.613	16.917	1.00 16.55	Α	0
ATOM	2235	N	ALA	306	36.064	71.484	15.704	1.00 16.10	Α	N
ATOM	2236	CA	ALA	306	34.661	71.620	16.079	1.00 17.20	A	Ç
ATOM	2237	CB	ALA	306	34. 336	73.074	16.384	1.00 18.47	A	C
ATOM	2238	С	ALA.		33. 770	71.110	14.956	1.00 16.79	A	C
ATOM	2239	0	ALA	306	32. 829	70.369	15. 191	1.00 18.46	A	0 N
ATOM	2240	N	THR	307	34.076	71.516	13. 733	1.00 18.36	A A	N C
ATOM	2241	CA	THR	307	33. 314	71. 100	12. 564	1.00 18.83 1.00 18.43	A	Č
ATOM	2242	CB	THR	307	32. 387 33. 178	72. 222 73. 254	12. 072 11. 473	1.00 10.43	A	Ö
ATOM	2243	0G1	THR THR	307 307	31. 593	72. 811	13. 225	1.00 26.70	A	Č
ATOM ATOM	2244 2245	C	THR	307	34. 299	70. 778	11.442	1.00 20.34	Ä	Č
ATOM	2246	Ö	THR	307	35. 494	70. 626	11.689	1.00 22.05	A	0
ATOM	2247	N	GLN	308	33. 798	70. 688	10. 213	1.00 20.11	Α	N
ATOM	2248	CA	GLN	308	34. 640	70. 389	9.066	1.00 19.71	Α	C
ATOM	2249	CB	GLN	308	33. 799	69.942	7.866	1.00 19.44	A	Ç
ATOM	2250		GLN	308	32.845	68. 791	8. 118	1.00 21.53	A	C
ATOM	2251	CD	GLN	308	33. 524	67. 505	8. 557	1.00 23.81	A	C
ATOM	2252			308	32.854	66. 565	9.003	1.00 25.80	Ą	0
ATOM	2253	NE 2	GLN	308	34. 848	67. 449	8. 430	1.00 21.04	A	N

				•	(Continued)
				FIG. 4-47	,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2254 2255 2256 2257 2258 2259 2260 2261 2262 2263 2264 2265 2266 2270 2271 2272 2273 2274 2275 2277 2278 2277 2278 2279 2280 2281 2282 2283 2284 2285 2288 2289 2290 2291 2292 2293 2294 2295	C GLN O GLU CA GLU CB	308 308 309 309 309 309 309 310 310 310 310 311 311 311 311 311 311	35. 440 71. 616 8. 653 1. 00 19. 98 36. 421 71. 501 7. 922 1. 00 21. 84 35. 022 72. 789 9. 114 1. 00 19. 41 35. 710 74. 019 8. 751 1. 00 20. 93 34. 920 74. 764 7. 685 1. 00 21. 98 34. 709 73. 971 6. 419 1. 00 26. 38 33. 890 74. 731 5. 413 1. 00 29. 11 33. 665 74. 192 4. 305 1. 00 31. 98 33. 471 75. 869 5. 736 1. 00 28. 78 35. 924 74. 939 9. 932 1. 00 21. 37 36. 075 76. 152 9. 764 1. 00 21. 97 35. 941 74. 360 11. 125 1. 00 20. 65 36. 133 75. 131 12. 340 1. 00 20. 50 34. 779 75. 445 12. 986 1. 00 19. 87 34. 888 76. 186 14. 305 1. 00 22. 38 33. 519 76. 630 14. 786 1. 00 21. 66 32. 952 77. 605 13. 870 1. 00 20. 43 31. 660 77. 884 13. 785 1. 00 19. 88 30. 794 77. 261 14. 569 1. 00 21. 42 31. 235 78. 776 12. 902 1. 00 21. 69 37. 009 74. 346 13. 304 1. 00 19. 05 36. 701 73. 214 13. 671 1. 00 20. 19 38. 108 74. 959 13. 710 1. 00 17. 41 40. 371 73. 991 13. 859 1. 00 17. 28 40. 982 75. 252 13. 305 1. 00 14. 23 41. 358 73. 254 14. 765 1. 00 17. 79 42. 589 72. 763 14. 011 1. 00 15. 43 39. 283 75. 258 15. 802 1. 00 17. 06 39. 461 74. 692 16. 988 1. 00 19. 09 39. 008 74. 173 20. 074 1. 00 18. 57 41. 084 75. 269 18. 736 1. 00 19. 09 39. 008 74. 173 20. 074 1. 00 18. 57 41. 084 75. 269 18. 736 1. 00 19. 07 43. 080 76. 271 19. 708 1. 00 20. 08 44. 093 76. 301 18. 768 1. 00 19. 07 44. 239 76. 409 17. 341 1. 00 20. 02 45. 480 77. 038 16. 712 1. 00 19. 82 44. 361 74. 892 17. 351 1. 00 20. 74	C C C C C C C C C C C C C C C C C C C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2296 2297 2298 2299 2300 2301	CDZ LEU C LEU N GLN CA GLN CB GLN CG GLN	313 313 314 314 314 314	43. 172 76. 957 21. 062 1. 00 21. 08 42. 608 78. 030 21. 265 1. 00 21. 22 43. 898 76. 333 21. 981 1. 00 22. 23 44. 096 76. 884 23. 308 1. 00 22. 40 43. 545 75. 935 24. 365 1. 00 24. 62 43. 545	A C A O A N A C A C
ATOM	2302	CD GLN	314		A C

							(Continued)
					FIG. 4-48		(Oondinaca)
•							
ATOM	2303	0E1		314	41. 827 74. 911 26. 598		A O
ATOM	2304	NE2		314	40.786 73.854 24.911		A N
ATOM	2305	C	GLN	314	45. 584 77. 099 23. 532		A C
ATOM	2306	0	GLN	314	46. 382 76. 176 23. 419		A O A N
ATOM	2307	N	TRP	315	45. 954 78. 333 23. 833 47. 343 78. 667 24. 070		A C
ATOM	2308	CA CB	TRP TRP	315 315	47. 748 79. 873 23. 226		A C
ATOM ATOM	2309 2310	CG	TRP	315	47. 480 79. 711 21. 746		A Č
ATOM	2311	CD2		315	48. 435 79. 368 20. 733		A Č
ATOM	2312	CE2		315	47. 764 79. 419 19. 491		A Č
ATOM	2313	CE3		315	49. 793 79. 029 20. 753		A C
ATOM	2314	CD1	TRP	315	46. 299 79. 936 21. 095		A C
ATOM	2315	NE 1		315	46. 463 79. 769 19. 742		A N
ATOM	2316	CZ2		315	48. 407 79. 147 18. 278		A C
ATOM	2317	CZ3		315	50. 433 78. 760 19. 545	1.00 13.87	A C
ATOM	2318	CH2		315	49. 736 78. 822 18. 325	1.00 12.57	A C
ATOM	2319	C	TRP	315	47. 530 78. 976 25. 545		A C
ATOM	2320	0	TRP	315	46.615 79.463 26.205		A 0
ATOM	2321	N	LEU	316	48. 721 78. 689 26. 056		A N
ATOM	2322	CA	LEU	316	49. 033 78. 915 27. 458		A C
ATOM	2323	CB	LEU	316	49. 034 77. 573 28. 192		A C
ATOM	2324	CG	LEU	316	49. 655 77. 484 29. 584		A C
ATOM	2325		LEU	316	48. 953 78. 438 30. 530		A C
ATOM	2326		LEU	316	49. 557 76. 049 30. 085		A C
ATOM	2327	C	LEU	316	50. 383 79. 617 27. 618		A C
ATOM	2328	0	LEU	316	51. 392 79. 192 27. 046 50. 388 80. 704 28. 383		A O
ATOM	2329	N	ARG	317			A N A C
ATOM	2330	CA	ARG	317 317	51.603 81.475 28.630 51.265 82.787 29.337		A C A C
ATOM ATOM	2331 2332	CB CG	ARG ARG	317	50.490 83.785 28.504		A C
ATOM	2333	CD	ARG	317	50. 187 85. 012 29. 327		A C
ATOM	2334	NE	ARG	317	49. 796 86. 141 28. 494		A N
ATOM	2335	CZ	ARG	317	49. 278 87. 269 28. 966		Ä Č
ATOM	2336	NH1	ARG	317	49. 082 87. 414 30. 273		A N
ATOM	2337		ARG	317	48. 972 88. 256 28. 132		A N
ATOM	2338	C	ARG	317	52. 580 80. 705 29. 500		A C
ATOM	2339	0	ARG	317	52. 175 79. 920 30. 359		A 0
ATOM	2340	N	ARG	318	53. 871 80. 941 29. 290		A N
ATOM	2341	CA	ARG	318	54. 876 80. 259 30. 084	1.00 17.08	A C
ATOM	2342	CB	ARG	318	56. 263 80. 850 29. 845		A C
ATOM	2343	CG	ARG	318	57. 345 80. 075 30. 564		A C
ATOM	2344	CD	ARG	318	58. 671 80. 165 29. 853		A C
ATOM	2345	NE	ARG	318	59. 687 79. 341 30. 504		A N
ATOM	2346	CZ	ARG	318	60. 895 79. 135 30. 001		A C
ATOM	2347		ARG	318	61. 220 79. 694 28. 850		A N
ATOM	2348		ARG	318	61. 773 78. 378 30. 642		A N
ATOM	2349	C	ARG	318	54. 500 80. 354 31. 555		A C.
ATOM	2350	0	ARG	318	54. 794 79. 448 32. 318		A O
ATOM	2351	N	ILE	319	53.869 81.455 31.954	1.00 16.59	A N

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		(Continued)
F I G. 4 - 49		(00110111111011)
ATOM 2352 CA ILE 319 53.396 81.607 33.330 1.00 17.40 ATOM 2353 CB ILE 319 53.389 83.078 33.776 1.00 17.03 ATOM 2354 CG2 ILE 319 52.720 83.210 35.128 1.00 17.19 ATOM 2355 CG1 ILE 319 54.828 83.589 33.878 1.00 19.57 ATOM 2356 CD1 ILE 319 55.712 82.743 34.787 1.00 19.56 ATOM 2357 C ILE 319 51.972 81.065 33.251 1.00 17.56 ATOM 2358 O ILE 319 51.012 81.808 33.067 1.00 18.71 ATOM 2359 N GLN 320 51.870 79.747 33.381 1.00 16.94 ATOM 2360 CA GLN 320 50.623 79.001 33.246 1.00 16.12 ATOM 2361 CB GLN 320 50.939 77.516 33.420 1.00 14.59 ATOM 2362 CG GLN 320 52.000 77.044 32.444 1.00 12.17	A A A A A A A A A A	C C C C C O N C C C
ATOM 2363 CD GLN 320 52.304 75.577 32.570 1.00 10.79 ATOM 2364 OE1 GLN 320 51.431 74.734 32.403 1.00 12.70 ATOM 2365 NE2 GLN 320 53.554 75.261 32.860 1.00 13.71	A A A	C O N
ATOM 2366 C GLN 320 49.368 79.351 34.038 1.00 16.32 ATOM 2367 O GLN 320 48.645 78.466 34.472 1.00 14.51 ATOM 2368 N ASN 321 49.079 80.633 34.207 1.00 18.37 ATOM 2369 CA ASN 321 47.871 81.010 34.931 1.00 19.38	A A A	C O N C
ATOM 2370 CB ASN 321 48. 226 81. 785 36. 203 1. 00 20. 21 ATOM 2371 CG ASN 321 48. 776 83. 166 35. 925 1. 00 23. 59 ATOM 2372 OD1 ASN 321 49. 166 83. 491 34. 804 1. 00 22. 35	A A A	C C O
ATOM 2373 ND2 ASN 321 48.801 83.975 36.980 1.00 27.82 ATOM 2374 C ASN 321 46.983 81.843 34.020 1.00 18.69 ATOM 2375 O ASN 321 46.095 82.555 34.479 1.00 19.10	A A A	N C O
ATOM 2376 N TYR 322 47. 222 81. 715 32. 719 1. 00 17. 65 ATOM 2377 CA TYR 322 46. 482 82. 466 31. 719 1. 00 18. 28 ATOM 2378 CB TYR 322 47. 105 83. 856 31. 599 1. 00 18. 09	A A A	N C C
ATOM 2379 CG TYR 322 46. 319 84. 856 30. 792 1. 00 20. 14 ATOM 2380 CD1 TYR 322 46. 561 85. 037 29. 428 1. 00 21. 33 ATOM 2381 CE1 TYR 322 45. 843 85. 987 28. 694 1. 00 22. 14	A A	C C C
ATOM 2382 CD2 TYR 322 45.340 85.645 31.401 1.00 20.00 ATOM 2383 CE2 TYR 322 44.624 86.589 30.681 1.00 19.18 ATOM 2384 CZ TYR 322 44.876 86.758 29.334 1.00 21.74 ATOM 2385 OH TYR 322 44.163 87.704 28.638 1.00 24.04	A A A	C C C
ATOM 2386 C TYR 322 46.518 81.750 30.363 1.00 18.70 ATOM 2387 O TYR 322 47.583 81.587 29.764 1.00 18.36 ATOM 2388 N SER 323 45.351 81.318 29.896 1.00 17.43	A A A	C O N
ATOM 2389 CA SER 323 45. 237 80. 638 28. 612 1. 00 17. 45 ATOM 2390 CB SER 323 44. 871 79. 163 28. 806 1. 00 16. 45 ATOM 2391 OG SER 323 43. 662 79. 025 29. 535 1. 00 17. 51	A A A	C C O
ATOM 2392 C SER 323 44.163 81.320 27.777 1.00 17.88 ATOM 2393 O SER 323 43.250 81.943 28.314 1.00 18.20 ATOM 2394 N VAL 324 44.277 81.199 26.461 1.00 18.44 ATOM 2395 CA VAL 324 43.309 81.802 25.555 1.00 18.83	A A A	C O N C C
ATOM 2396 CB VAL 324 43.925 82.995 24.800 1.00 19.32 ATOM 2397 CG1 VAL 324 42.944 83.509 23.760 1.00 18.46 ATOM 2398 CG2 VAL 324 44.290 84.105 25.785 1.00 18.78 ATOM 2399 C VAL 324 42.839 80.776 24.534 1.00 18.47 ATOM 2400 0 VAL 324 43.631 79.985 24.036 1.00 18.75	A A A A	C C C O

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					E T	G. 4	- 50			(Con	tinued)
					гі	G. 4	- 50				
ATOM	2401		MET	325	41.549	80.772	24. 231	1.00 17.		N	
ATOM	2402		MET	325	41.046	79.832	23. 245	1.00 17.		C	
ATOM	2403		MET	325	39. 832	79.062	23.769	1.00 19.		C	
ATOM	2404		MET	325	39. 272	78.043	22.774	1.00 20.		C	
ATOM	2405		MET	325	37.681	77. 304	23. 268	1.00 23.		S	
ATOM	2406		MET	325	38. 209	75. 734	23.896	1.00 24.		C	
ATOM	2407		MET	325	40.641	80. 584	21.999	1.00 18.		C 0	
ATOM	2408		MET	325	39. 932	81.583	22.076	1.00 16. 1.00 18.		N N	
ATOM	2409		ASP	326	41.114	80.118	20.852			C	
ATOM	2410		ASP	326	40.749	80. 738	19.595	1.00 20. 1.00 22.		C	
ATOM	2411		ASP	326	41.988	81. 158 82. 638	18. 797 18. 970	1.00 22.		Č	
ATOM	2412		ASP	326	42. 329 41. 511		19.547	1.00 26.		Õ	
ATOM	2413	OD1		326	43.415	83. 063	18.518	1.00 28.		ŏ	
ATOM	2414	OD2 C		326 326	39. 924		18.800	1.00 20.		č	
ATOM	2415		ASP ASP	326	40. 254		18.729	1.00 21.		ő	
ATOM ATOM	2416 2417		ILE	327	38. 832	80. 208	18. 223	1.00 20.		Ň	
ATOM	2418		ILE	327	37. 980	79. 355	17.419	1.00 22.		Ċ	
ATOM	2419	CB	ILE	327	36. 529	79. 393	17. 941	1.00 20.		č	
ATOM	2420	CG2		327	35. 600	78. 697	16.985	1.00 19.		č	
ATOM	2421	CG1		327	36. 483	78. 691	19.305	1.00 21.		č	
ATOM	2422	CD1		327	35. 164		20.006	1.00 20.		. Č	
ATOM	2423	C	ILE	327	38. 113		16.015	1.00 23.		Č	
ATOM	2424	Ŏ	ILE	327	37.625		15.716	1.00 26.		0	
ATOM	2425	N	CYS	328	38.804		15.161	1.00 26.	09 A	N	
ATOM	2426	CA	CYS	328	39.069	79.608	13.805	1.00 26.	75 A	C	
ATOM	2427	C	CYS	328	38.274	78.890	12.721	1.00 27.		C	
ATOM	2428	0	CYS	328	38.168		12.705	1.00 27.		0	
ATOM	2429	CB	CYS	328	40.564		13.547	1.00 27.		C	
ATOM	2430	SG	CYS	328	41.567		14.986	1.00 28.		S	
ATOM	2431	N	ASP	329	37. 729		11.807	1.00 26.		N	
ATOM	2432		ASP	329	36. 913		10.710	1.00 26.		C	
ATOM	2433	CB	ASP	329 ·	35. 595		10.690	1.00 24.		C	
ATOM	2434	CG	ASP	329	34.684		11.842	1.00 26.		C	
ATOM	2435		ASP	329	35. 181	79. 407	12.969	1.00 27.		0	
ATOM	2436		ASP	329	33. 460		11.625	1.00 28.		0	
ATOM		C			37.613			1.00 28.	54 A		
ATOM	2438	0	ASP	329	38. 314		9.120	1.00 29.		0 N	
ATOM	2439	N	TYR	330	37.416	78.371	8.492	1.00 29. 1.00 29.		N C	
ATOM	2440	CA	TYR	330	38. 027 38. 011	78.411	7.173	1.00 29.		C	
ATOM	2441	CB	TYR	330	38. 597	77. 019 76. 980	6.542	1.00 30.		C	
ATOM	2442	CG	TYR	330	39.919	77. 367	5. 151 4. 919	1.00 31.		C	
ATOM	2443		TYR	330	40. 460	77. 341	3. 641	1.00 32.		Č	
ATOM	2444		TYR TYR	330 330	37. 832	76. 561	4.066	1.00 32.		Č	
ATOM	2445 2446		TYR	330 330	38. 364		2. 779	1.00 32.		Č	
ATOM	2440	CZ	TYR	330 330	39. 676		2. 574	1.00 32.		Č	
ATOM ATOM	2448	OH	TYR	330	40. 193		1. 299	1.00 34.		ŏ	
ATOM	2449	C	TYR	330	37. 314		6. 243	1.00 30.		Č	
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(Continued)

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					FI	G. 4	- 51			
ATOM	2450	0	TYR	330	36.098	79.313	6.058	1.00 28.65	Α	0
ATOM	2451	Ň	ASP	331	38. 074	80.308	5.666	1.00 31.49	Α	N
ATOM	2452	ĊA	ASP	331	37. 511	81.262	4.730	1.00 33.80	Α	C
ATOM	2453	CB	ASP	331	38. 191	82.618	4.862	1.00 36.63	Α	C
ATOM	2454	CG	ASP	331	37. 573	83.661	3.956	1.00 39.35	Α	C
ATOM	2455	0D1		331	37. 570	83. 455	2.724	1.00 40.70	Α	0
ATOM	2456		ASP	331	37. 084	84.684	4.479	1.00 42.41	Α	0
ATOM	2457	C	ASP	331	37.750	80.696	3.336	1.00 35.29	Α	C
ATOM	2458	Ō	ASP	331	38.865	80.730	2.817	1.00 35.63	Α	0
ATOM	2459	N	GLU	332	36.690	80.170	2.743	1.00 36.11	Α	N
ATOM.	2460	CA	GLU	332	36.755	79.562	1.426	1.00 37.77	Α	C
ATOM	2461	CB	GLU	332	35.388	78.970	1.080	1.00 38.87	A	C
ATOM	2462	CG .	GLU	332	35.234	78.510	-0.354	1.00 43.60	A	C
ATOM	2463	CD	GLU	332	33.869	77.897	-0.620	1.00 47.15	A	C
ATOM	2464		GLU	332	33.494	77.771	-1.807	1.00 48.97	A	0
ATOM	2465		GLU	332	33. 175	77.534	0.358	1.00 48.40	A	0
ATOM	2466	C	GLU	332	37. 231	80.465	0. 293	1.00 38.19	A	C
ATOM	2467	0	GLU	332	37. 846	79. 982	-0.655	1.00 39.73	A	0
ATOM	2468	N	SER	333	36. 968	81.764	0.375	1.00 37.67	A	N
ATOM	2469	CA	SER	333	37. 388	82.652	-0.704	1.00 38.09 1.00 38.48	A	C
ATOM	2470	CB	SER	333 333	36. 445	83. 858 84. 795	-0.814 0.223	1.00 38.48	A A	0
ATOM	$\frac{2471}{2472}$	OG C	SER SER	333	36. 669 38. 826	83. 135	-0.577	1.00 40.00	A	C
ATOM ATOM	2473	0	SER	333	39. 324	83. 838	-0.377	1.00 31.14	A	Ö
ATOM	2474	N .	SER	334	39. 496	82. 761	0.506	1.00 38.49	A	N
ATOM	2475	CA	SER	334	40. 883	83. 163	0.708	1.00 37.49	A	Ċ
ATOM	2476	CB	SER	334	40.995	84. 180	1.844	1.00 38.50	Ä	č
ATOM	2477	0G	SER	334	40. 954	83. 536	3. 108	1.00 38.48	Ä	ŏ
ATOM	2478	Č	SER	334	41.722	81.947	1.058	1.00 35.98	Ā	Č
ATOM	2479	Ŏ	SER	334	42. 941	82.029	1.148	1.00 36.41	Ā	Ō
ATOM	2480	N	GLY	335	41.064	80.817	1.263	1.00 35.13	A	N
ATOM	2481	CA	GLY	335	41.797	79.620	1.620	1.00 35.71	Α	С
ATOM	2482	C	GLY	335	42.579	79.872	2.894	1.00 35.19	Α	C
ATOM	2483	0	GLY	335	43. 574	79. 201	3.172	1.00 35.61	A	0
ATOM	2484	N	ARG	336	42. 128	80.855	3.666	1.00 33.99	A	'N
ATOM	2485	CA	ARG	336	42. 783	81. 197	4.919	1.00 33.15	Α	С
ATOM	2486	CB	ARG	336	43.066	82.696	4.991	1.00 36.78	A	C
ATOM	2487	CG	ARG	336	43.957	83. 232	3.884	1.00 42.04	A	C
ATOM	2488	CD	ARG	336	44.807	84. 374	4.416	1.00 45.76	A	C
ATOM	2489	NE	ARG	336	44.010	85. 359	5. 147	1.00 48.92	A	N
ATOM	2490	CZ	ARG	336	44. 510	86. 192	6.055	1.00 50.76	A	C
ATOM	2491	NH1	ARG	336	45. 805	86. 159	6.348	1.00 52.08	A	N
ATOM	2492		ARG	336	43.718	87.057	6.675	1.00 52.33	A	N
ATOM	2493	C	ARG	336	41.935	80. 801	6.118	1.00 30.26	A	C
ATOM ATOM	2494 2495	0 N	ARG TRP	336 337	40.763	80.449	5. 981 7. 294	1.00 29.07 1.00 26.94	A A	O N
	2495 2496	CA	TRP	337	42. 544 41. 869	80. 869 80. 531	8. 533	1. 00 20. 94	A	C
ATOM ATOM	2490	CB	TRP	337	41.809	79. 403	9. 248	1.00 24.29	A	C
ATOM	2498	CG	TRP	337	42. 460	78. 074	8. <u>56</u> 1	1.00 15.00	A	č
VIÓN	<i>4</i> 730	UU	III	501	,44.400	10.014	0.7001	1.00 10.10	Λ	J

				FIG. 4-52	(Continued)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2499 2500 2501 2502 2503 2504 2505 2506 2507 2518 2511 2512 2513 2514 2515 2516 2517 2518 2519 2520 2521 2522 2523 2524 2525 2524 2525 2526 2527 2528 2529 2530 2531 2532 2532 2533 2534 2532 2533 2534 2535 2536 2536 2537 2538 2538 2538 2538 2538 2538 2538 2538	CD2 TRP CE2 TRP CE3 TRP CD1 TRP NE1 TRP CZ2 TRP CZ3 TRP CH2 TRP O TRP N ASN CA ASN CB ASN CB ASN CG ASN ND2 ASN C ASN C CYS C	337 337 337 337 337 337 337 338 338 338	FIG. 4 - 5 2 41.481 77.077 8.861 1.00 9.80 A 41.651 76.026 7.927 1.00 9.92 A 40.475 76.970 9.825 1.00 7.74 A 43.173 77.601 7.485 1.00 12.90 A 42.688 76.369 7.099 1.00 9.82 A 40.849 74.885 7.935 1.00 9.71 A 39.675 75.836 9.832 1.00 7.79 A 39.866 74.808 8.894 1.00 10.33 A 41.783 81.758 9.425 1.00 24.55 A 42.794 82.360 9.766 1.00 26.73 A 40.570 82.128 9.806 1.00 25.00 A 40.381 83.296 10.648 1.00 26.17 A 39.464 84.300 9.949 1.00 28.44 A 40.016 84.761 8.612 1.00 30.42 A 40.016 84.761 8.612 1.00 32.04 A 41.271 85.217 8.606 1.00 28.33 A 41.271 85.217 8.606 1.00 28.33 A 39.810 82.958 12.012 1.00 25.29 A 40.293 83.668 13.023 1.00 25.00 A 40.293 83.668 13.023 1.00 25.00 A 39.833 83.482 14.389 1.00 24.73 A 39.289 84.829 14.888 1.00 22.42 A 40.051 85.717 15.249 1.00 21.56 A 40.992 83.014 15.285 1.00 25.93 A 42.199 81.865 14.526 1.00 29.61 A 37.968 84.978 14.889 1.00 22.38 A 37.333 86.212 15.347 1.00 20.83 A 35.899 86.85 15.069 1.00 19.89 A 35.899 86.85 15.069 1.00 19.21 A 33.877 85.883 13.593 1.00 19.65 A 37.366 87.625 17.225 1.00 20.46 A 37.337 85.478 17.615 1.00 20.80 A 37.366 87.625 17.225 1.00 20.46 A 38.966 87.949 18.627 1.00 20.11 A 38.536 89.399 18.786 1.00 21.45 A 39.688 89.672 17.819 1.00 21.45 A 39.688 89.672 17.819 1.00 21.45 A 38.972 89.647 20.221 1.00 22.38 A 39.688 89.672 17.819 1.00 24.23	CCCCNCCCONCCONCCONCCONCCCCCCONCCCC
ATOM ATOM	2535 2536 2537 2538	CG2 VAL C VAL O VAL N ALA	341 341 341 342	39. 588 89. 672 17. 819 1. 00 24. 28 A 36. 770 87. 749 19. 403 1. 00 18. 51 A 36. 785 87. 423 20. 585 1. 00 17. 77 A 35. 644 87. 941 18. 731 1. 00 19. 68 A	C O N
ATOM ATOM ATOM ATOM	2539 2540 2541	CA ALA CB ALA C ALA O ALA	342 342 342 342 342	34. 345 87. 756 19. 370 1. 00 19. 64 A 33. 228 88. 125 18. 407 1. 00 18. 89 A 34. 177 86. 302 19. 829 1. 00 19. 19 A 33. 245 85. 987 20. 580 1. 00 18. 12 A	C C C O
ATOM ATOM ATOM ATOM ATOM	2542 2543 2544 2545 2546	N ARG CA ARG CB ARG CG ARG	343 343 343 343	35. 078 85. 422 19. 384 1. 00 16. 06 A 35. 008 84. 017 19. 766 1. 00 16. 37 A 34. 962 83. 138 18. 521 1. 00 18. 14 A 33. 726 83. 390 17. 687 1. 00 20. 31 A	N C C C
ATOM	2547	CD ARG	343	33. 803 82. 695 16. 357 1. 00 21. 82 A	U

(Continued)

				1 7	G. 4	- 53			(Co
4 TO 1 F	05.40	NID AI	0.40				1.00 23.94	٨	N
ATOM	2548		RG 343 RG 343	32. 615 32. 373	82. 969 82. 415	15. 561 14. 383	1.00 25.34	A A	Č
ATOM	2549	CZ AI NH1 AI		33. 242	81.559	13. 864	1.00 28.42	A	N
ATOM ATOM	2550 2551	NH2 Al		31. 256	82. 703	13.734	1.00 20.42	A	N
ATOM	2552		RG 343	36.164	83.603	20.650	1.00 17.09	A	Č
ATOM	2553		RG 343	36. 275	82. 452	21.057	1.00 16.76	Ä	ŏ
ATOM	2554		LN 344	37. 030	84. 553	20.955	1.00 18.05	Ä	Ň
ATOM	2555		LN 344	38. 175	84. 267	21.791	1.00 18.90	A	C
ATOM	2556		LN 344	39. 191	85.385	21.645	1.00 18.03	Α	C
ATOM	2557		LN 344	40.585	85.012	22.038	1.00 17.99	Α	C
ATOM	2558	CD G	LN 344	41.571	86.088	21.657	1.00 18.02	Α	С
ATOM	2559	OE1 G		41.711	87. 089	22. 353	1.00 17.71	A	0
ATOM	2560	NE2 G		42. 246	85. 897	20. 527	1.00 17.42	Ą	N
ATOM	2561		LN 344	37. 708	84.170	23. 234	1.00 19.61	A	Ç
ATOM	2562		LN 344	37.069	85.087	23. 730	1.00 21.89	A	0
ATOM	2563		IS 345	38.013	83.057	23. 897	1.00 18.47	A	N C
ATOM	2564 2565		IS 345 IS 345	37. 624 36. 786	82.868 81.600	25. 287 25. 453	1.00 17.92 1.00 16.07	A A	C
ATOM ATOM	2566	CG H		35. 478	81.641	24. 726	1.00 15.01	A	č
ATOM	2567	CD2 H		34. 223	81.895	25. 164	1.00 14.43	A	č
ATOM	2568	ND1 H		35. 371	81.420	23. 369	1.00 15.56	Ä	Ň
ATOM	2569	CE1 H		34. 108	81.535	23.002	1.00 12.57	A	C
ATOM	2570	NE2 H		33.390	81.823	24.073	1.00 14.20	Α	N
ATOM	2571		IS 345	38.854	82. 789	26. 172	1.00 19.64	Α	C
ATOM	2572		IS 345	39. 839	82.129	25. 825	1.00 22.18	A	0
ATOM	2573		LE 346	38. 790	83.460	27. 319	1.00 20.11	A	N
ATOM	2574		LE 346	39. 899	83. 501	28. 264	1.00 21.08	A	C
ATOM	2575		LE 346	40. 135	84. 928	28. 760 29. 667	1.00 20.44 1.00 20.95	A	C
ATOM ATOM	2576 2577	CG2 II		41. 357 40. 338	84. 972 85. 860	27. 572	1.00 20.93	A A	C
ATOM	2578	CD1 I		40. 466	87. 298	27. 978	1.00 22.20	A	Č
ATOM	2579		LE 346	39.657	82. 624	29. 482	1.00 23.76	Ä	č
ATOM	2580		LE 346	38. 535	82. 537	29. 975	1.00 24.67	Ä	ŏ
ATOM	2581		LU 347	40. 714	81.976	29.967	1.00 25.01	A	Ň
ATOM	2582	CA G	LU 347	40.601	81.123	31.141	1.00 28.30	Α	C
ATOM	2583		LU 347	40. 459	79.656	30. 733	1.00 26.51	Α	C
ATOM	2584		LU 347		78. 740		1.00 27.38	Α	C
ATOM	2585		LU 347	40. 169	77. 268	31.527	1.00 29.51	Ą	C
ATOM	2586	OE1 G		39. 877	76. 936	30. 359	1.00 29.48	A	0
ATOM	2587	OE2 G		40. 511	76. 439	32. 405	1.00 29.57	A	0
ATOM	2588		LU 347	41.836	81. 288	32.021	1.00 30.87	A	C
ATOM	2589 2590		LU 347 ET 348	42.865 41.741	80.661	31.777 33.044	1. 00 33. 35 1. 00 32. 50	A A	0 M
ATOM ATOM	2591		ET 348	42.877	82. 131 82. 347	33. 926	1.00 32.30	A	N C
ATOM	2592		ET 348	43. 215	83. 843	34. 002	1.00 37.48	A	C
ATOM	2593		ET 348	42. 168	84. 723	34.661	1.00 41.62	Ä	č
ATOM	2594		ET 348	42.028	86. 340	33. 825	1. 00 48. 03	Ä	Š
ATOM	2595		ET 348	43.541	87. 158	34. 341	1.00 46.60	A	Č
ATOM	2596	C M	ET 348	42.628	81.784	35. 315	1.00 33.55	A	C

					(Continued)
				FIG. 4-54	•==
ATOM ATOM ATOM ATOM ATOM ATOM	2597 2598 2599 2600 2601 2602 2603	O MET N SER CA SER CB SER OG SER C SER O SER N THR	348 349 349 349 349 349 349 350	41. 656 81. 070 35. 541 1. 00 34. 35 A 43. 534 82. 085 36. 235 1. 00 32. 30 A 43. 428 81. 623 37. 612 1. 00 31. 26 A 43. 961 80. 197 37. 744 1. 00 31. 22 A 43. 912 79. 760 39. 090 1. 00 32. 92 A 44. 244 82. 573 38. 474 1. 00 31. 16 A 45. 355 82. 950 38. 113 1. 00 31. 25 A 43. 682 82. 962 39. 611 1. 00 30. 83	0 N C C O C O N
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2604 2605 2606 2607 2608 2609 2610 2611	N THR CA THR CB THR OG1 THR CG2 THR C THR O THR N THR	350 350 350 350 350 350 350	44. 340 83. 896 40. 516 1. 00 28. 43 A 43. 325 84. 938 41. 027 1. 00 28. 93 A 42. 251 84. 268 41. 703 1. 00 27. 68 A 42. 751 85. 733 39. 864 1. 00 27. 87 A 44. 971 83. 198 41. 714 1. 00 27. 14 A 45. 781 83. 786 42. 431 1. 00 27. 62 A 44. 610 81. 936 41. 913 1. 00 25. 72	C C O C C O N
ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2612 2613 2614 2615 2616 2617 2618	CA THR CB THR OG1 THR CG2 THR C THR O THR N GLY	351 351 351 351 351 351 352	45. 109 81. 161 43. 035 1. 00 24. 77 A 43. 945 80. 536 43. 786 1. 00 25. 52 A 43. 166 79. 746 42. 877 1. 00 24. 95 A 43. 069 81. 617 44. 385 1. 00 24. 61 A 46. 081 80. 047 42. 659 1. 00 25. 48 A 46. 648 79. 392 43. 535 1. 00 25. 57 A 46. 261 79. 825 41. 361 1. 00 25. 19 A	C C O C C O N
ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2619 2620 2621 2622 2623 2624 2625	CA GLY C GLY O GLY N TRP CA TRP CB TRP CG TRP	352 352 352 353 353 353 353	47. 170 78. 786 40. 909 1. 00 24. 62 A 47. 371 78. 797 39. 403 1. 00 24. 61 A 47. 417 79. 853 38. 774 1. 00 25. 15 A 47. 499 77. 612 38. 825 1. 00 23. 36 A 47. 684 77. 470 37. 390 1. 00 21. 38 A 48. 631 76. 291 37. 116 1. 00 17. 49 A 48. 272 75. 023 37. 849 1. 00 16. 34 A	C C O N C C C
ATOM ATOM ATOM ATOM ATOM ATOM	2626 2627 2628 2629 2630 2631 2632	CD2 TRP CE2 TRP CE3 TRP CD1 TRP NE1 TRP CZ2 TRP CZ3 TRP	353 353 353 353 353 353 353	48. 587 74. 693 39. 209 1. 00 14. 04 A 48. 053 73. 409 39. 462 1. 00 14. 33 A 49. 270 75. 356 40. 238 1. 00 14. 55 A 47. 578 73. 957 37. 351 1. 00 14. 89 A 47. 445 72. 985 38. 311 1. 00 12. 84 A 48. 180 72. 768 40. 709 1. 00 14. 93 A 49. 398 74. 719 41. 480 1. 00 15. 27 A	C C C N C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2633 2634 2635 2636 2637 2638	CH2 TRP C TRP O TRP N VAL CA VAL CB VAL	353 353 353 354 354 354	48. 853 73. 436 41. 700 1. 00 15. 07 A 46. 303 77. 236 36. 782 1. 00 22. 43 A 45. 307 77. 292 37. 495 1. 00 22. 69 A 46. 231 76. 990 35. 479 1. 00 22. 83 A 44. 944 76. 749 34. 836 1. 00 24. 15 A 44. 818 77. 513 33. 498 1. 00 25. 09 A	C C O N C C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2639 2640 2641 2642 2643 2644 2645	CG2 VAL C VAL O VAL N GLY CA GLY	354 354 354 354 355 355 355	43. 610 77. 006 32. 718 1. 00 24. 29 A 44. 673 79. 007 33. 762 1. 00 24. 71 A 44. 799 75. 264 34. 569 1. 00 24. 96 A 45. 751 74. 628 34. 127 1. 00 26. 10 A 43. 609 74. 722 34. 841 1. 00 24. 28 A 43. 354 73. 303 34. 640 1. 00 22. 67 A 44. 040 72. 457 35. 696 1. 00 22. 77 A	C C O N C

					((Continued)
				FIG. 4-55		
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2646 2647 2648 2649 2650 2652 2653 2655 2655 2656 2666 2666 2666	O GLY N ARG CA ARG CB ARG CCB ARG CCD ARG NE ARG CZ ARG NH1 ARG C ARG N PHE CA PHE CA PHE CCB PHE CCD1 PHE CCD2 PHE CCD2 PHE CCD2 PHE CCD2 PHE CCD2 PHE CCD2 PHE CCD3 PHE CCD4 PHE CCD4 PHE CCD6 PHE CCD7 PHE CCD7 PHE CCD7 PHE CCD7 PHE CCD7 PHE CCD7 PHE CCCC PHE CCCCC PHE CCCC PHE CCC	355 356 356 356 356 356 356 356 357 357 357 357 357 357 357 357 357 358 358 358	43. 843 71. 145 35. 668 1. 00 23. 29 44. 505 70. 299 36. 654 1. 00 24. 86 43. 927 68. 886 36. 645 1. 00 24. 91 42. 495 68. 808 37. 122 1. 00 27. 84 41. 973 67. 391 37. 036 1. 00 31. 58 40. 518 67. 340 37. 149 1. 00 35. 53 39. 849 67. 607 38. 261 1. 00 37. 59 40. 513 67. 939 39. 362 1. 00 40. 39 38. 520 67. 547 38. 272 1. 00 37. 65 45. 989 70. 255 36. 314 1. 00 25. 60 46. 844 70. 508 37. 163 1. 00 28. 06 46. 285 69. 940 35. 060 1. 00 23. 61 47. 659 69. 876 34. 587 1. 00 21. 95 48. 029 68. 442 34. 205 1. 00 15. 99 48. 173 67. 524 35. 380 1. 00 12. 89 49. 361 67. 491 36. 115 1. 00 11. 73 47. 126 66. 693 35. 763 1. 00 10. 46 49. 507 66. 638 37. 216 1. 00 7. 55 47. 263 65. 838 36. 863 1. 00 11. 70 48. 459 65. 811 37. 591 1. 00 6. 24 47. 775 70. 786 33. 377 1. 00 23. 17 48. 877 71. 196 33. 005 1. 00 26. 25 46. 626 71. 100 32. 782 1. 00 20. 84 46. 541 71. 972 31. 615 1. 00 20. 05 47. 156 71. 297 30. 396 1. 00 19. 30 46. 496 69. 991 30. 011 1. 00 21. 15	A A A A A A A A A A A A A A A A A A A	
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2670 2671 2672 2673 2674 2675 2676 2677 2678 2689 2681 2682 2683 2684 2685 2686 2687 2688	CA ARG CB ARG CC ARG NE ARG CZ ARG NH1 ARG NH2 ARG C ARG O ARG N PRO CD PRO CA PRO CC	358	46. 541 71. 972 31. 615 1. 00 20. 05 47. 156 71. 297 30. 396 1. 00 19. 30	A A	C C
ATOM ATOM ATOM ATOM ATOM ATOM	2689 2690 2691 2692 2693 2694		360 360 360 360 361 361	39. 501 70. 986 30. 497 1. 00 25. 25 38. 505 71. 976 30. 283 1. 00 27. 66 40. 262 71. 280 28. 140 1. 00 25. 67 40. 117 72. 359 27. 555 1. 00 25. 66 40. 024 70. 104 27. 573 1. 00 25. 65 39. 581 69. 972 26. 199 1. 00 27. 20	A A A A	O C O N C

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			٠.		(Continued)
				FIG. 4-56	(Commueu)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2695 2696 2697 2698 2699 2700 2701 2702 2703 2704 2705 2706	CB GLU CG GLU OE1 GLU OE2 GLU C GLU O GLU N PRO CD PRO CA PRO CG PRO	361 361 361 361 361 361 362 362 362 362	39. 803 68. 540 25. 713 1. 00 30. 37 A 39. 356 67. 444 26. 683 1. 00 36. 42 A 40. 340 67. 226 27. 839 1. 00 42. 80 A 40. 317 68. 002 28. 822 1. 00 43. 77 A 41. 152 66. 274 27. 757 1. 00 46. 60 A 38. 112 70. 324 26. 052 1. 00 25. 88 A 37. 295 69. 955 26. 888 1. 00 27. 12 A 37. 760 71. 061 24. 989 1. 00 23. 97 A 38. 650 71. 837 24. 106 1. 00 23. 33 A 36. 365 71. 436 24. 767 1. 00 22. 45 A 36. 485 72. 714 23. 945 1. 00 23. 21 A 37. 679 72. 437 23. 100 1. 00 21. 08	C C C O N C C C C C
ATOM ATOM ATOM	2707 2708 2709	C PRO O PRO N HIS	362 362 363	35. 621 70. 338 24. 013 1. 00 21. 91 A 36. 216 69. 582 23. 249 1. 00 22. 96 A 34. 318 70. 259 24. 245 1. 00 21. 59 A	C O N
ATOM ATOM ATOM ATOM	2710 2711 2712 2713	CA HIS CB HIS CG HIS CD2 HIS	363 363 363	33. 459 69. 280 23. 596 1. 00 19. 88 A 32. 868 68. 353 24. 649 1. 00 18. 03 A 33. 898 67. 568 25. 398 1. 00 16. 56 A 34. 638 67. 880 26. 489 1. 00 16. 19 A	C C C C
ATOM ATOM ATOM ATOM	2714 2715 2716 2717	NDI HIS CE1 HIS NE2 HIS C HIS	363 363 363 363	34. 292 66. 303 25. 019 1. 00 14. 56 A 35. 227 65. 869 25. 843 1. 00 14. 60 A 35. 457 66. 808 26. 744 1. 00 16. 65 A 32. 364 70. 081 22. 903 1. 00 20. 84 A	N C N C
ATOM ATOM ATOM ATOM	2718 2719 2720 2721	O HIS N PHE CA PHE CB PHE	363 364 364 364	31. 535 70. 709 23. 564 1. 00 20. 84 A 32. 383 70. 075 21. 573 1. 00 19. 87 A 31. 416 70. 832 20. 786 1. 00 18. 84 A 32. 042 71. 310 19. 470 1. 00 18. 67 A	O N C C
ATOM ATOM ATOM ATOM	2722 2723 2724 2725	CG PHE CD1 PHE CD2 PHE CE1 PHE	364 364 364 364	33.073 72.390 19.629 1.00 18.84 A 34.341 72.096 20.117 1.00 17.51 A 32.776 73.708 19.274 1.00 16.76 A 35.298 73.095 20.246 1.00 16.92 A	C C C
ATOM ATOM ATOM ATOM ATOM	2726 2727 2728 2729 2730	CE2 PHE CZ PHE C PHE O PHE N THR	364 364 364 364 365	33. 727 74. 711 19. 401 1. 00 16. 24 A 34. 988 74. 404 19. 886 1. 00 16. 59 A 30. 172 70. 046 20. 432 1. 00 19. 35 A 30. 226 68. 831 20. 262 1. 00 20. 71 A 29. 050 70. 750 20. 313 1. 00 18. 81 A	C C C O N
ATOM ATOM ATOM ATOM	2731 2732 2733 2734	CA THR CB THR OG1 THR CG2 THR	365 365 365 365	27. 805 70. 113 19. 912 1. 00 18. 11 A 26. 600 71. 017 20. 161 1. 00 17. 38 A 26. 521 71. 991 19. 119 1. 00 22. 40 A 26. 741 71. 734 21. 487 1. 00 13. 72 A	C C O C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2735 2736 2737 2738 2739 2740 2741 2742 2743	C THR O THR N LEU CA LEU CB LEU CG LEU CD1 LEU CD2 LEU C LEU C LEU	365 365 366 366 366 366 366 366	28. 001 69. 954 18. 409 1. 00 17. 58 A 28. 823 70. 650 17. 824 1. 00 16. 70 A 27. 250 69. 058 17. 784 1. 00 19. 74 A 27. 388 68. 799 16. 350 1. 00 19. 89 A 26. 237 67. 923 15. 860 1. 00 19. 49 A 26. 338 67. 381 14. 431 1. 00 19. 63 A 27. 606 66. 542 14. 282 1. 00 20. 45 A 25. 112 66. 539 14. 128 1. 00 17. 80 A 27. 503 70. 017 15. 438 1. 00 21. 11	C O N C C C C

				FIG. 4-57	(Continued)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2744 2745 2746 2747 2748 2749 2750 2751 2752 2753 2754 2755 2756 2757 2762 2761 2762 2763 2764 2765 2766 2767 2768 2769 2770 2771 2772 2773 2774 2775 2776 2777 2778 2777	O LEU N ASP CA ASP CB ASP OD1 ASP OD2 ASP OD2 ASP OD3 ASP C GLY O GLY O GLY O ASN CA ASN CB ASN CG ASN CB ASN CC A	366 367 367 367 367 367 367 367 368 368 369 369 369 369 369 369 370 370 370 370 371 371 371 371 371 371	28. 269 69. 989 14. 476 1. 00 24. 21 26. 764 71. 084 15. 722 1. 00 21. 26 26. 830 72. 261 14. 867 1. 00 22. 95 25. 567 73. 114 15. 005 1. 00 26. 09 25. 458 73. 796 16. 355 1. 00 29. 82 26. 469 73. 849 17. 094 1. 00 28. 76 24. 352 74. 296 16. 669 1. 00 31. 88 28. 047 73. 130 15. 139 1. 00 22. 76 28. 818 72. 772 16. 155 1. 00 21. 02 30. 001 73. 541 16. 480 1. 00 18. 54 29. 740 74. 946 16. 987 1. 00 17. 42 30. 678 75. 690 17. 237 1. 00 17. 82 28. 482 75. 324 17. 164 1. 00 17. 57 28. 196 76. 669 17. 647 1. 00 17. 82 26. 838 77. 129 17. 144 1. 00 17. 82 26. 797 77. 234 15. 649 1. 00 22. 41 27. 657 77. 871 15. 038 1. 00 23. 56 25. 798 76. 606 15. 038 1. 00 23. 56 25. 798 76. 606 15. 038 1. 00 26. 52 28. 270 76. 838 19. 158 1. 00 16. 27 28. 185 77. 949 19. 665 1. 00 16. 44 28. 432 75. 742 19. 882 1. 00 15. 67 28. 533 75. 824 21. 330 1. 00 16. 34 27. 145 75. 766 21. 971 1. 00 14. 45 26. 523 74. 518 21. 739 1. 00 14. 37 29. 381 74. 660 21. 797 1. 00 16. 66 29. 565 73. 701 21. 058 1. 00 18. 15 29. 910 74. 742 23. 014 1. 00 17. 09 30. 735 73. 660 23. 532 1. 00 16. 28 32. 194 73. 808 23. 062 1. 00 14. 83 32. 881 75. 062 23. 546 1. 00 11. 31 32. 799 76. 243 22. 818 1. 00 11. 07 33. 635 75. 050 24. 726 1. 00 11. 89 33. 465 77. 409 23. 256 1. 00 12. 04 34. 302 76. 205 25. 178 1. 00 9. 92 34. 219 77. 383 24. 444 1. 00 9. 76	A O N A C C A A C C A A A A A A A A A A A A
ATOM ATOM ATOM	2780 2781 2782	C PHE O PHE N TYR	371 371 372	30. 703 73. 545 25. 048 1. 00 16. 26 30. 362 74. 495 25. 752 1. 00 15. 15 31. 053 72. 360 25. 536 1. 00 16. 67	A C A O A N
ATOM ATOM ATOM ATOM ATOM	2784 2785 2786 2787	CA TYR CB TYR CG TYR CD1 TYR CE1 TYR	372 372 372 372 372	31. 091 72. 089 26. 962 1. 00 16. 84 30. 349 70. 801 27. 271 1. 00 16. 79 28. 892 70. 879 26. 914 1. 00 18. 47 28. 470 70. 744 25. 589 1. 00 16. 97 27. 129 70. 850 25. 255 1. 00 19. 91	A C A C A C A C A C
ATOM ATOM ATOM ATOM ATOM	2789 2790 2791	CD2 TYR CE2 TYR CZ TYR OH TYR C TYR	372 372 372 372 372	27. 931 71. 124 27. 901 1. 00 18. 26 26. 592 71. 235 27. 581 1. 00 19. 23 26. 193 71. 097 26. 258 1. 00 21. 51 24. 860 71. 210 25. 944 1. 00 23. 32 32. 547 71. 977 27. 367 1. 00 18. 35	A C A C A C A O A C

									(Continued)
				F-I	G. 4	- 58			,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,
ATOM ATOM ATOM ATOM ATOM ATOM	2793 2794 2795 2796 2797 2798	O TY N LY CA LY CB LY CG LY CD LY	S 373 S 373 S 373 S 373	33. 388 32. 845 34. 224 34. 907 36. 302 36. 658	71.557 72.325 72.318 73.541 73.863 75.193	26. 571 28. 611 29. 071 28. 459 28. 889 28. 240	1.00 20.30 1.00 18.89 1.00 19.69 1.00 19.69 1.00 20.48 1.00 23.59	A A A A	O N C C C C
ATOM ATOM	2799 2800	CE LY NZ LY	S 373 S 373	38. 048 38. 103	75. 703 77. 196	28. 601 28. 404	1.00 25.15 1.00 24.26	A A	C N
ATOM ATOM ATOM	2801 2802 2803	C LY O LY N IL	S 373 E 374	34. 277 33. 474 35. 215	72. 369 73. 050 71. 634	30. 593 31. 231 31. 176 32. 621	1.00 20.26 1.00 21.08 1.00 20.43	A A A	C O . N C
ATOM ATOM ATOM	2804 2805 2806	CA IL CB IL CG2 IL	E 374 E 374	35. 358 35. 960 36. 100	71. 624 70. 309 70. 361	33. 123 34. 650	1.00 19.63 1.00 19.72 1.00 19.46	A A A	C C
ATOM ATOM ATOM	2807 2808 2809	CG1 IL CD1 IL C IL	E 374 E 374	35. 095 35. 652 36. 290	69. 128 67. 753 72. 745	32. 667 33. 079 33. 046	1.00 19.17 1.00 15.57 1.00 19.75	A A A	C C C
ATOM ATOM ATOM	2810 2811 2812	0 IL N IL CA IL	E 375 E 375	37. 408 35. 824 36. 643	72. 846 73. 595 74. 684	32. 551 33. 951 34. 456	1.00 21.23 1.00 20.12 1.00 20.15	A A A	O N C
ATOM ATOM ATOM	2813 2814 2815	CB IL CG2 IL CG1 IL	E 375	36. 396 36. 685 34. 966	76. 014 75. 837 76. 488	33. 700 32. 215 33. 919	1.00 20.38 1.00 20.24 1.00 20.36	A A A	C C C
ATOM ATOM ATOM	2816 2817 2818	CD1 IL C IL O IL	E 375 E 375	34. 645 36. 346 35. 283	77. 772 74. 893 74. 512	33. 186 35. 929 36. 426	1.00 21.00 1.00 21.63 1.00 21.72	A A A	C C O
ATOM ATOM ATOM	2819 2820 2821	N SE CA SE CB SE	R 376 R 376	37. 301 37. 132 38. 449	75. 481 75. 740 76. 228	36. 634 38. 051 38. 632	1.00 22.04 1.00 23.67 1.00 21.76	A A A	N C C
ATOM ATOM	2822 2823	OG SE C SE	R 376 R 376	38. 336 36. 063	76. 411 76. 809	40. 022 38. 210	1.00 26.97 1.00 24.46	A A	C 0
ATOM ATOM ATOM	2824 2825 2826	O SE N AS CA AS	N 377 N 377	36. 042 35. 164 34. 128	77. 768 76. 659 77. 673	37. 445 39. 177 39. 356	1.00 27.59 1.00 25.41 1.00 26.19	A A A	O N C
ATOM ATOM ATOM	2827 2828 2829	CB AS CG AS OD1 AS	N 377	32. 755 32. 682 33. 560	77. 023 76. 222 76. 294	39. 602 40. 894 41. 750	1.00 25.06 1.00 22.15 1.00 23.03	A A A	C C 0
ATOM ATOM ATOM	2830 2831 2832	ND2 AS C AS O AS	N 377	31.606 34.447 35.574	75. 457 78. 685 78. 733	41.039 40.456 40.960	1.00 20.01 1.00 28.48 1.00 29.51	A A A	N C O
ATOM ATOM ATOM	2833 2834 2835	N GL CA GL CB GL	U 378 U 378	33. 461 33. 659 32. 401	79. 498 80. 518 81. 390	40. 822 41. 845 41. 988	1.00 30.42 1.00 33.25 1.00 36.97	A A A	N C C
ATOM ATOM ATOM	2836 2837 2838	CG GL CD GL OE1 GL	U 378 U 378	32. 300 31. 099 29. 946	82. 505 83. 430 82. 970	40. 939 41. 148 40. 972	1.00 44.33 1.00 49.20 1.00 51.65	A A A	C C O
ATOM ATOM ATOM	2839 2840 2841	OE2 GL C GL O GL	U 378 U 378	31. 312 34. 065 34. 582	84. 619 79. 975 80. 718	41. 489 43. 208 44. 040	1.00 50.97 1.00 32.75 1.00 33.80	A A A	0 C 0
UIOII	POTI	v 0L		07.004	00.110	11.010	1.00 00.00	п	V

						(Continued)
				FIG. 4-59		(Continuou)
				•		
ATOM	2842	N GLU	379	00.012	A	N C
ATOM	2843	CA GLU	379	01.102	A A	C C
ATOM	2844	CB GLU	379	00.000	A	C
ATOM	2845	CG GLU	379		Ä	č
ATOM	2846	CD GLU OE1 GLU	379 379		Ä	Ŏ
ATOM ATOM	2847 2848	OE2 GLU	379		Ä	0
ATOM	2849	C GLU	379		A	С
ATOM	2850	0 GLU	379	35. 952 76. 712 45. 578 1. 00 30. 56	A	0
ATOM	2851	N GLY	380	35. 986 77. 136 43. 373 1. 00 29. 06	A	Ŋ
ATOM	2852	CA GLY	380	01.200	A	C
ATOM	2853	C GLY	380	00.010	A	C
ATOM	2854	O GLY	380	011000 121201	A A	O N
ATOM	2855	N TYR	381		A	C
ATOM	2856	CA TYR CB TYR	381 381	35. 434 73. 167 42. 191 1. 00 26. 78 34. 175 72. 671 42. 903 1. 00 26. 62	A	Č
ATOM ATOM	2857 2858	CB TYR	381	34. 394 72. 448 44. 379 1. 00 24. 99	A	C C C
ATOM	2859	CD1 TYR	381	34.864 71.225 44.853 1.00 24.93	Α	С
ATOM	2860	CE1 TYR	381	35. 145 71. 035 46. 204 1. 00 26. 71	Α	C
ATOM	2861	CD2 TYR	381	34. 202 73. 486 45. 296 1. 00 25. 27	A	Č
ATOM	2862	CE2 TYR	381	34. 480 73. 312 46. 647 1. 00 26. 88	A	C
ATOM	2863	CZ TYR	381	34. 955 72. 082 47. 097 1. 00 28. 08	A	C
ATOM	2864	OH TYR	381	35. 266 71. 909 48. 429 1. 00 28. 31	A	0 0
ATOM	2865	C TYR	381	35. 261 73. 100 40. 678 1. 00 26. 94 34. 542 73. 911 40. 091 1. 00 28. 94	A A	0
ATOM	2866	O TYR	381 382	34. 542 73. 911 40. 091 1. 00 28. 94 35. 938 72. 147 40. 045 1. 00 24. 97	A	N
ATOM ATOM	2867 2868	N ARG CA ARG	382	35. 855 72. 003 38. 600 1. 00 22. 04	Ä	č
ATOM	2869	CB ARG	382	37.057 71.211 38.081 1.00 24.10	Ä	Č
ATOM	2870	CG ARG	382	38. 322 72. 045 38. 110 1. 00 24. 01	A	C
ATOM	2871	CD ARG	382	39.606 71.237 38.141 1.00 24.10	A	С
ATOM	2872	NE ARG	382	40.647 72.083 38.712 1.00 23.35	A	N
ATOM	2873	CZ ARG	382	41.178 73.132 38.096 1.00 23.31	A	Ç
ATOM	2874	NH1 ARG	382	40. 783 73. 449 36. 868 1. 00 21. 52	A	N
ATOM	2875	NH2 ARG	382	42. 052 73. 907 38. 738 1. 00 22. 46	A	N
ATOM	2876	C ARG	382	34. 548 71. 359 38. 186 1. 00 20. 92 34. 189 70. 270 38. 645 1. 00 18. 12	A A	C 0
MOTA	2877 2878	O ARG N HIS	382 383	34. 189 70. 270 38. 645 1. 00 18. 12 33. 840 72. 068 37. 313 1. 00 20. 45	A	N N
ATOM ATOM	2879	N HIS CA HIS	383	32.545 71.647 36.813 1.00 20.33	A	Ċ
ATOM	2880	CB HIS	383	31. 440 72. 370 37. 581 1. 00 20. 76	Ä	Č
ATOM	2881	CG HIS	383	31. 177 71. 797 38. 939 1. 00 22. 34	Α	С
ATOM	2882	CD2 HIS	383	31.590 72.189 40.168 1.00 21.75	Α	С
ATOM	2883	ND1 HIS	383	30.418 70.661 39.132 1.00 20.42	A	N
ATOM	2884	CE1 HIS	383	30. 374 70. 380 40. 422 1. 00 22. 91	A	C
ATOM	2885	NE2 HIS	383	31. 076 71. 291 41. 073 1. 00 22. 25	A	N
ATOM	2886	C HIS	383	32.404 71.930 35.330 1.00 20.36	A	C 0
ATOM	2887	0 HIS	383	33. 240 72. 608 34. 728 1. 00 19. 84 31. 325 71. 420 34. 748 1. 00 19. 26	A A	O N
ATOM	2888	N ILE CA ILE	384 384		A	C
ATOM ATOM	2889 2890		384	31. 078 71. 589 33. 329 1. 00 17. 93 30. 232 70. 419 32. 802 1. 00 17. 52	Ä	č
VION	2030	OD IEE	004	00. 202 10. 110 02. 002 1. 00 11. 02	••	-

FIG. 4-60											
ATOM ATOM	2891 2892	CG2 ILE	384 384	30.928 6	0.566 9.097	31. 290 33. 155	1. 00 15. 28 1. 00 12. 97	A A	C C		
ATOM ATOM	2893 2894	CD1 ILE C ILE	384 384	30.376 7	7. 865 2. 898	32. 909 33. 028	1.00 9.57 1.00 19.30	A A	C .		
ATOM	2895	0 ILE	384	29.333 7	3. 198	33.605	1.00 18.50	A	0 N		
ATOM ATOM	2896 2897	N CYS CA CYS	385 385		'3. 681 '4. 953	32. 120 31. 745	1.00 21.14 1.00 24.26	A A	N C		
ATOM	2898	C CYS	385	29.932 7	4.887	30. 284	1.00 23.62	A	С		
ATOM	2899	0 CYS	385		4.334	29.464	1.00 23.61	A	0		
ATOM ATOM	2900 2901	CB CYS SG CYS	385 385		'6. 106 '7. 640	31.958 32.569	1.00 27.85 1.00 37.75	A A	C S		
ATOM	2902	N TYR	386	28.760 7	5. 440	29.973	1.00 23.26	Ä	N		
ATOM	2903	CA TYR	386		5. 470	28. 609	1.00 21.88	A	C		
ATOM ATOM	2904 2905	CB TYR CG TYR	386 386		5. 271 5. 183	28. 612 27. 228	1.00 21.89 1.00 23.48	A A	C C		
ATOM	2906	CD1 TYR	386	24.912 7	5. 825	26.930	1.00 23.55	A	č		
ATOM	2907	CE1 TYR	386		5.712	25.665	1.00 24.11	A	C		
ATOM ATOM	2908 2909	CD2 TYR CE2 TYR	386 386		4. 424 4. 299	26. 223 24. 956	1.00 22.70 1.00 23.04	A A	C C		
ATOM	2910	CZ TYR	386		4. 946	24. 686	1.00 24.39	A	č		
ATOM	2911	OH TYR	386		4. 823	23. 449	1.00 23.13	A	0		
ATOM ATOM	2912 2913	C TYR O TYR	386 386		6. 816 7. 868	27. 962 28. 493	1.00 22.02 1.00 22.52	A A	C 0		
ATOM	2914	N PHE	387		6. 775	26. 806	1.00 21.19	A	N		
ATOM	2915	CA PHE	387	29.582 7	7.988	26.080	1.00 19.95	Α	C		
ATOM ATOM	2916 2917	CB PHE	387 387		7. 987 8. 222	25. 781 26. 973	1.00 17.05 1.00 14.01	A	C C C C		
ATOM	2918	CD1 PHE	387		9.469	27. 185	1.00 14.01	A A	C		
ATOM	2919	CD2 PHE	387	32. 293 7	7.178	27.835	1.00 11.20	Α	Č		
ATOM ATOM	2920 2921	CE1 PHE CE2 PHE	387 387		9. 672 7. 376	28. 231 28. 885	1.00 9.80	A	C		
ATOM	2922	CZ PHE	387	33. 762 7	8. 626	29. 082	1.00 10.91 1.00 9.32	A A	C		
ATOM	2923	C PHE	387	28.888 7	8. 153	24.727	1.00 20.94	A	C		
ATOM	2924	0 PHE	387		7. 180	24. 055	1.00 19.77	A	0		
ATOM ATOM	2925 2926	N GLN CA GLN	388 388		9. 406 9. 742	24. 332 23. 030	1.00 21.79 1.00 22.21	A A	N C		
ATOM	2927	CB GLN	388		0.760	23. 177	1.00 23.86	Ä	C		
ATOM	2928	CG GLN	388		0.343	22.477	1.00 29.81	A	C		
ATOM ATOM	2929 2930	CD GLN OE1 GLN	388 388		9. 126 8. 391	23. 109 ° 22. 452	1.00 32.86 1.00 34.98	A A	C 0		
ATOM	2931	NE2 GLN	388		8. 913	24. 395	1.00 34.36	A	N		
ATOM	2932	C GLN	388		0. 382	22.427	1.00 21.72	A	C		
ATOM ATOM	2933 2934	O GLN N ILE	388 389		1. 428 9. 745	22. 893 21. 415	1.00 22.74 1.00 20.66	A	0 N		
ATOM	2935	CA ILE	389		0. 215	20. 821	1.00 20.00	A A	N C		
ATOM	2936	CB ILE	389	31.466 7	9.617	19. 422	1.00 20.76	Α	C		
MOTA	2937	CG2 ILE	389 380		8. 100	19.496	1.00 19.50	A	C		
ATOM ATOM	2938 2939	CG1 ILE CD1 ILE	389 389		0. 165 9. 864	18. 429 16. 992	1.00 19.48 1.00 19.12	A A	C C		
			-						-		

										(Continued)
					FI	G. 4	6 1			
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2940 2941 2942 2943 2944 2945 2946 2947 2948	O	ILE ASP ASP ASP ASP ASP ASP	389 389 390 390 390 390 390 390 390	31. 483 32. 640 30. 423 30. 584 29. 932 28. 467 27. 754 28. 029 30. 005	81. 713 82. 146 82. 505 83. 953 84. 508 84. 215 84. 955 83. 236 84. 676	20. 735 20. 776 20. 611 20. 533 19. 275 19. 216 18. 517 19. 858 21. 738	1. 00 23. 29 1. 00 22. 48 1. 00 24. 96 1. 00 26. 49 1. 00 29. 09 1. 00 30. 91 1. 00 35. 45 1. 00 33. 49 1. 00 26. 43	A A A A A A	C O N C C C O O
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2949 2950 2951 2952 2953 2954 2955 2956 2957	N I CA I CB I CC I CC I CC I CC I CC I CC	ASP LYS LYS LYS LYS LYS LYS LYS LYS	390 391 391 391 391 391 391 391 391	29. 402 30. 163 29. 707 28. 348 27. 203 25. 867 24. 733 23. 454 30. 772	85. 735 84. 078 84. 679 84. 128 84. 790 84. 228 84. 772 84. 073 84. 369	21, 603 22, 910 24, 150 24, 566 23, 824 24, 256 23, 413 23, 742 25, 183	1.00 26.54 1.00 27.05 1.00 28.81 1.00 28.62 1.00 31.00 1.00 34.06 1.00 33.69 1.00 36.51 1.00 29.11	A A A A A A A	O N C C C C C C C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2958 2959 2960 2961 2962 2963 2964 2965	O N CA CB CC CC CC	LYS LYS LYS LYS LYS LYS LYS LYS	391 392 392 392 392 392 392 392 392	31. 192 31. 219 32. 281 33. 069 33. 516 34. 330 34. 643 35. 369	83. 223 85. 401 85. 248 86. 558 87. 119 86. 098 86. 588 87. 872	25. 327 25. 888 26. 872 26. 985 25. 636 24. 852 23. 449 23. 495	1. 00 29. 45 1. 00 29. 66 1. 00 30. 67 1. 00 28. 28 1. 00 27. 07 1. 00 27. 55 1. 00 26. 02 1. 00 25. 63	A A A A A A A	O N C C C C C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2966 2967 2968 2969 2970 2971 2972 2973	C O N CA CB	LYS LYS ASP ASP ASP ASP ASP	392 392 393 393 393 393 393 393	31. 824 32. 637 30. 531 30. 015 29. 052 29. 734 30. 607 29. 409	84. 797 84. 679 84. 548 84. 098 85. 134 86. 450 86. 475 87. 455	28. 248 29. 162 28. 403 29. 690 30. 271 30. 567 31. 467 29. 895	1.00 31.24 1.00 32.17 1.00 31.57 1.00 33.64 1.00 36.88 1.00 41.66 1.00 43.84 1.00 44.39	A A A A A A	C O N C C C O
ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2974 2975 2976 2977 2978 2979 2980	C O N CA C O CB	ASP ASP CYS CYS CYS CYS CYS	393 393 394 394 394 394 394	29. 309 28. 294 29. 841 29. 243 28. 312 28. 262 30. 336	82. 761 82. 666 81. 731 80. 410 80. 116 80. 858 79. 338 79. 166	29. 546 28. 859 30. 198 30. 115 31. 282 32. 258 30. 033 31. 504	1. 00 32. 46 1. 00 32. 91 1. 00 30. 05 1. 00 28. 94 1. 00 27. 56 1. 00 27. 11 1. 00 31. 03 1. 00 34. 42	A A A A A A	C O N C C O C S
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2981 2982 2983 2984 2985 2986 2987 2988	N CA CB OG1 CG2	CYS THR THR THR THR THR THR THR	394 395 395 395 395 395 395 395	31. 401 27. 570 26. 645 25. 208 24. 709 24. 289 27. 048 27. 196	79. 166 79. 023 78. 608 78. 512 79. 833 77. 779 77. 251 76. 280	31. 167 32. 204 31. 647 31. 407 32. 620 32. 772 32. 036	1.00 34.42 1.00 25.71 1.00 25.01 1.00 25.50 1.00 28.36 1.00 21.52 1.00 24.22 1.00 24.44	A A A A A A	N . C C O C C C

					FΙ	G. 4	- 62			(Continued)
ATOM	2989	. И	PHE	396	27. 231	77. 185	34. 084	1.00 23.09	Α	N
ATOM	2990	CA	PHE	396	27. 594	75. 924	34. 715	1.00 23.03	Α	C
ATOM	2991	CB	PHE	396	28. 138	76. 182	36. 116	1.00 22.19	Α	C
ATOM	2992	CG	PHE	396	29. 581	76.617	36. 131	1.00 23.20	A	Ċ
ATOM	2993		PHE	396	30.604	75.697	35. 876	1.00 22.48	A	Č
ATOM	2994		PHE	396	29. 924	77. 935	36. 415	1.00 20.97	A	C
ATOM	2995		PHE	396	31.949	76.086	35. 908	1.00 20.26	A	C
ATOM	2996		PHE	396	31. 267	78. 331	36. 447	1.00 21.70	. A	C
ATOM	2997	CZ	PHE	396	32. 279	77. 400	36. 194	1.00 20.27	A	C
ATOM	2998	C	PHE	396	26. 373	75.008	34. 764	1.00 20.96	A	C
ATOM ATOM	2999 3000	N. 0	PHE	396 397	25. 311 26. 523	75. 412 73. 779	35. 218	1.00 20.96	A	0
ATOM	3000	CA	ILE	397	25. 412	72. 842	34. 279 34. 262	1.00 18.88 1.00 18.00	A	N C
ATOM	3002	CB	ILE	397	25. 266	72. 165	32. 879	1.00 16.00	A	C
ATOM	3002		ILE	397	25. 350	73. 209	31. 787	1.00 10.55	A A	C
ATOM	3004		ILE	397	26. 366	71.130	32.669	1.00 16.03	A	C
ATOM	3005		ILE	397	26. 180	70. 327	31.402	1.00 17.85	A	C C C C
ATOM	3006	C	ILE	397	25. 527	71.770	35. 338	1.00 19.16	A	Ç
ATOM	3007	ŏ	ILE	397	24. 787	70. 787	35. 330	1.00 20.44	A	ŏ
ATOM	3008	Ň	THR	398	26. 480	71.956	36. 244	1.00 18.55	A	Ň
ATOM	3009	CA	THR	398	26. 681	71.051	37. 367	1.00 19.41	Ä	Ċ
ATOM	3010	CB	THR	398	27. 624	69.858	37. 051	1.00 19.56	A	č
ATOM	3011	0G1	THR	398	28.978	70.321	36.960	1.00 22.60	A	Ö
ATOM	3012	CG2	THR	398	27. 221	69.178	35.759	1.00 18.50	Ä	Č
ATOM	3013	C	THR	398	27. 343	71.899	38. 424	1.00 20.24	A	Ċ
ATOM	3014	0	THR	398	27.979	72.903	38.104	1.00 20.11	A	0
ATOM	3015	N	LYS	399	27. 185	71.511	39.681	1.00 22.48	A	N
ATOM	3016	CA	LYS	399	27. 795	72. 258	40.772	1.00 23.72	A	C
ATOM	3017	CB	LYS	399	27.111	73.618	40.941	1.00 24.42	Α	C ·
ATOM	3018	CG	LYS	399	25. 689	73. 583	41.462	1.00 27.65	Α	С
ATOM	3019	CD	LYS	399	25. 269	74.996	41.856	1.00 30.77	Α	С
ATOM	3020	CE	LYS	399	23. 861	75.054	42.414	1.00 31.89	Α	C
ATOM	3021	NZ	LYS	399	22. 841	74. 747	41.377	1.00 35.03	A	N
ATOM	3022	C	LYS	399	27. 751	71.476	42.077	1.00 22.46	A	Č
ATOM	3023	0	LYS	399	27. 125	70. 425	42. 154	1.00 21.96	A	0
ATOM	3024	N	GLY	400	28. 435	71. 989	43.093	1.00 21.98	A	N
ATOM	3025	CA	GLY	400	28. 463	71.319	44. 378	1.00 22.66	A	C
ATOM ATOM	3026 3027	C 0	GLY GLY	400 400	29. 891	71.115	44. 839	1.00 24.94	A	C
ATOM	3028	N	THR	400	30. 831	71.449	44. 118	1.00 26.10	A	0
ATOM	3029	CA	THR	401	30. 064 31. 400	70. 566 70. 335	46.036	1.00 25.34	A	N
ATOM	3030	CB	THR	401	31.443	70. 541	46.560	1.00 26.41	A	C
ATOM	3031		THR	401	30.615	69. 567	48. 095 48. 741	1.00 27.75 1.00 31.37	A A	C
ATOM	3032		THR	401	30. 924	71. 927	48. 448	1.00 31.37	A A	0
ATOM	3033	C	THR	401	31. 923	68. 945	46. 197	1.00 24.83	A	C C
ATOM	3034	ŏ	THR	401	32. 027	68. 049	47. 036	1.00 24.03	A	0
ATOM	3035	Ň	TRP	402	32. 229	68. 790	44. 915	1.00 22.03	A	N
ATOM	3036	CA	TRP	402	32. 781	67. 569	44. 340	1.00 18.83	A	Č
ATOM	3037	CB	TRP	402	31.741	66.460	44. 268	1.00 16.39	Ä	Č

				FIG. 4-63		(Continued)
ATOM	3038	CG TRP	402	30. 434 66. 886 43. 709 1. 00 17. 90	A	С
ATOM	3039	CD2 TRP	402	30. 037 66. 865 42. 332 1. 00 19. 16	A	č
ATOM	3040	CE2 TRP	402	28. 701 67. 320 42. 278 1. 00 20. 21	Ä	č
ATOM	3041	CE3 TRP	402	30.679 66.505 41.137 1.00 18.78	Ä	č
ATOM	3042	CD1 TRP	402	29. 364 · 67. 345 44. 409 1. 00 17. 97	Ä	č
ATOM	3043	NE1 TRP	402	28.318 67.605 43.562 1.00 20.57	Ā	Ň
ATOM	3044	CZ2 TRP	402	27. 989 67. 425 41. 078 1. 00 18. 32	A	Ċ
ATOM	3045	CZ3 TRP	402	29.972 66.608 39.943 1.00 19.71	Α	C
ATOM	3046	CH2 TRP	402	28. 637 67. 064 39. 924 1. 00 18. 98	Α	С
ATOM	3047	C TRP	402	33. 208 67. 983 42. 944 1. 00 18. 09	Α	С
ATOM	3048	0 TRP	402	32.956 69.117 42.540 1.00 18.12	Α	0
ATOM	3049	N GLU	403	33. 831 67. 089 42. 191 1. 00 17. 78	A	N
ATOM	3050	CA GLU	403	34. 284 67. 484 40. 866 1. 00 19. 48	A	C
ATOM	3051	CB GLU	403	35. 776 67. 805 40. 926 1. 00 20. 26	A	C
ATOM	3052	CG GLU	403	36. 122 68. 824 41. 983 1. 00 21. 69	A	C
ATOM ATOM	3053 3054	CD GLU OE1 GLU	403	37. 433 69. 522 41. 721 1. 00 23. 95 37. 506 70. 728 42. 020 1. 00 25. 27	A	C
ATOM	3055	OE1 GLU	403 403		A	0
ATOM	3056	C GLU	403	38. 384 68. 880 41. 223 1. 00 24. 57 34. 028 66. 516 39. 716 1. 00 19. 74	A	0
ATOM	3057	0 GLU	403	33. 891 65. 305 39. 916 1. 00 19. 74	A	C
ATOM	3058	N VAL	404	33. 957 67. 073 38. 508 1. 00 18. 47	A A	O N
ATOM	3059	CA VAL	404	33.760 66.273 37.305 1.00 17.63	A	C
ATOM	3060	CB VAL	404	33.070 67.073 36.165 1.00 14.78	A	C
ATOM	3061	CG1 VAL	404	32. 974 66. 210 34. 914 1. 00 11. 14	A	Č
ATOM	3062	CG2 VAL	404	31.683 67.515 36.595 1.00 12.13	Ä	č
ATOM	3063	C · VAL	404	35. 153 65. 875 36. 836 1. 00 18. 38	Ä	č
ATOM	3064	0 VAL	404	35. 986 66. 732 36. 567 1. 00 20. 01	A	Ö
ATOM	3065	N ILE	405	35.410 64.579 36.764 1.00 18.83	Α	N
ATOM	3066	CA ILE	405	36.707 64.088 36.323 1.00 20.05	Α	C
ATOM	3067	CB ILE	405	36.868 62.593 36.653 1.00 21.78	Α	С
ATOM	3068	CG2 ILE	405	38. 254 62. 123 36. 283 1. 00 16. 28	Α	С
ATOM	3069	CG1 ILE	405	36. 591 62. 364 38. 146 1. 00 24. 51	Α	С
ATOM	3070	CD1 ILE	405	37. 438 63. 218 39. 079 1. 00 26. 24	Α	С
ATOM ATOM	3071	C ILE	405	36. 858 64. 290 34. 817 1. 00 19. 94	A	C
ATOM	3072 3073	O ILE N GLY	405 406	0 - 000 00 000 000 000 000	A	0
ATOM	3074	CA GLY	406	00 000 04 101 00 000 4 00 44 00	A	N
ATOM	3075	CA GLY	406	04 500 00 000 04 004	A	C
ATOM	3076	O GLY	406	00 450 00 000 00 000	A	C
ATOM	3077	N ILE	407	04 450 04 050 00 500 4 00 45	A	0
ATOM	3078	CA ILE	407	00 000 01 500 00 050	A	N
ATOM	3079	CB ILE	407	00 400 40 004 00 000	A A	C C
ATOM	3080	CG2 ILE	407		A	C
ATOM	3081	CG1 ILE	407		A	C
ATOM	3082	CD1 ILE	407	00 010 00 000 00 100 0 100	A	Č
ATOM	3083	C ILE	407	00 044 00 000 00 004	A	č
ATOM	3084	0 ILE	407	0.4 505 00 104 00 010	A	ŏ
ATOM	3085	N GLU	408	00 500 00 005 00 015 1 00 00	Ä	Ň
ATOM	3086	CA GLU	408	00 000 01 180 00 100 1 10 10 11	Ä	C

		٠.		FIG. 4-64		(Continued)
		an	400	•	A	C
ATOM	3087	CB GLU	408	32. 691 59. 922 28. 944 1. 00 21. 64	A	C
ATOM	3088	CG GLU	408	33. 457 59. 860 30. 254 1. 00 23. 48	A	C
ATOM	3089	CD GLU	408	34. 963 59. 947 30. 048 1. 00 26. 15	A	C
ATOM	3090	OE1 GLU	408	35.519 59.081 29.337 1.00 28.40	A	0
ATOM	3091	OE2 GLU	408	35. 594 60. 877 30. 596 1. 00 25. 87	A	0
ATOM	3092	C GLU	408	32. 262 61. 097 26. 780 1. 00 22. 35	A	C
ATOM	3093	O GLU	408	32.743 60.455 25.846 1.00 23.83	A	0
ATOM	3094	N ALA	409	31.100 61.729 26.671 1.00 22.21	A	N C
ATOM	3095	CA ALA	409	30.356 61.685 25.414 1.00 20.74	A	C
ATOM	3096	CB ALA	409	29.797 60.294 25.180 1.00 21.17	A	C
ATOM	3097	C ALA	409	29. 235 62. 708 25. 386 1. 00 20. 05	A	C
ATOM	3098	0 ALA	409	28. 651 63. 041 26. 413 1. 00 19. 39	A	0
ATOM	3099	N LEU	410	28. 937 - 63. 201 24. 195 1. 00 19. 25	A	N
ATOM	3100	CA LEU	410	27. 911 64. 207 24. 038 1. 00 19. 28	A	C
ATOM	3101	CB LEU	410	28, 559 65, 571 23, 796 1, 00 19, 29	A	C
ATOM	3102	CG LEU	410	27.634 66.778 23.617 1.00 20.83	A	C C
ATOM	3103	CD1 LEU	410	26.959 67.089 24.935 1.00 20.92	A	
ATOM	3104	CD2 LEU	410	28. 434 67. 987 23. 134 1. 00 20. 28 26. 998 63. 874 22. 879 1. 00 20. 25	A	C
ATOM	3105	C LEU	410	=	A	C
ATOM	3106	0 LEU	410	27. 453 63. 649 21. 758 1. 00 20. 84	A	0 N
ATOM	3107	N THR	411	25.701 63.834 23.150 1.00 19.86	A	N ·
ATOM	3108	CA THR	411	24.741 63.561 22.100 1.00 18.40	A	C
ATOM	3109	CB THR	411	23. 902 62. 339 22. 418 1. 00 15. 82	A	C
ATOM	3110	OG1 THR	411	23.017 62.649 23.498 1.00 15.79	A	0 C
ATOM	3111	CG2 THR	411	24.797 61.177 22.811 1.00 14.12	A	
ATOM	3112	C THR	411	23.846 64.787 22.050 1.00 20.16	A	C
ATOM	3113	0 THR	411	23. 971 65. 684 22. 882 1. 00 21. 79	A	0 N
ATOM	3114	N SER	412	22. 952 64. 836 21. 074 1. 00 20. 25	A	N
ATOM	3115	CA SER	412	22.061 65.972 20.945 1.00 21.09	A	C
ATOM	3116	CB SER	412	21. 206 65. 827 19. 687 1. 00 22. 27 20. 474 64. 618 19. 721 1. 00 25. 03	A	C 0
ATOM	3117	OG SER	412		A	C
ATOM	3118	C SER	412		A A	0
ATOM	3119	O SER	412	20. 598 67. 185 22. 379 1. 00 22. 97 21. 015 65. 054 22. 934 1. 00 22. 56	A	N
ATOM	3120	N ASP	413	20.138 65.104 24.097 1.00 24.36	Ā	Č
ATOM	3121	CA ASP	413		A	C
ATOM			413			Č
ATOM	3123	CG ASP	413		A A	Ö
ATOM	3124	OD1 ASP	413		A	0
ATOM	3125	OD2 ASP	413		A	C
ATOM	3126	C ASP	413		A	Ö
ATOM	3127	O ASP	413		A	N N
ATOM	3128	N TYR	414	21. 974 64. 259 25. 444 1. 00 24. 23 22. 672 63. 998 26. 694 1. 00 23. 03	A	C
ATOM	3129	CA TYR	414	22. 369 62. 572 27. 155 1. 00 23. 61	A	C
ATOM	3130	CB TYR CG TYR	414 414	20.925 62.332 27.520 1.00 25.79	A	C
ATOM	3131 3132	CG TYR CD1 TYR	414	20.402 62.822 28.714 1.00 26.31	A	Č
ATOM				= * · · · ·	A	Č
ATOM	3133	CE1 TYR	414		A	C
ATOM	3134	CD2 TYR	414		A	C
ATOM	3135	CE2 TYR	414	18.740 61.424 26.993 1.00 25.53	n	U

										(Continued)
					FΙ	G. 4	- 65			
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	3136 3137 3138 3139 3140 3141 3142 3143 3144 3145 3146 3147 3148	CA CB		414 414 414 415 415 415 415 415 415 416	18. 246 16. 925 24. 180 24. 811 24. 741 26. 174 26. 502 27. 945 28. 184 28. 208 26. 518 25. 926 27. 449	61. 923 61. 731 64. 174 64. 040 64. 469 64. 630 66. 079 66. 406 67. 892 65. 943 63. 684 63. 763 62. 769	28. 188 28. 531 26. 639 25. 582 27. 809 27. 996 28. 358 28. 745 28. 606 30. 163 29. 149 30. 230 28. 909	1. 00 28. 30 1. 00 31. 69 1. 00 22. 81 1. 00 22. 74 1. 00 20. 51 1. 00 18. 28 1. 00 16. 58 1. 00 14. 79 1. 00 13. 01 1. 00 14. 04 1. 00 18. 57 1. 00 18. 31 1. 00 19. 11	A A A A A A A A A A A A A A A A A A A	C O C O N C C C C C C
ATOM	3149	CA	TYR	416	27.843	61.796	29.924	1.00 19.69	Α	
ATOM ATOM ATOM	3150 3151 3152	CB CG CD1		416 416 416	27. 963 26. 698 26. 297	60.438	29. 309 28. 645 27. 410 26. 786	1.00 18.66 1.00 17.78 1.00 16.67 1.00 18.58	A A A	C C C C C
ATOM ATOM	3153 3154	CE1 CD2	TYR	416 416	25. 137 25. 908		29. 245	1.00 16.22	Α	C
ATOM ATOM	3155 3156	CE2 CZ	TYR TYR	416 416	24. 754 24. 374		28. 636 27. 406	1.00 16.35 1.00 18.54	• A	C C
ATOM	3157	0H	TYR TYR	416	23. 252 29. 167	58.489	26. 784 30. 540	1.00 19.53 1.00 20.71	A A	C 0
ATOM ATOM	3158 3159	0 C	TYR	416 416	30.117	62.499	29.822	1.00 22.92	Α	0
ATOM	3160	N CA	TYR TYR	417 417	29. 238 30. 472		31.866 32.544	1.00 19.27 1.00 19.08	A A	N C
ATOM ATOM	3161 3162	CB	TYR	417	30.408	63.981	32.970	1.00 18.38	Α	C
ATOM	3163	CG	TYR	417	29. 383	64. 282 64. 213	34. 049 35. 399	1.00 17.93 1.00 15.25	A A	C C
ATOM ATOM	3164 3165		TYR TYR	417 417	29. 721 28. 784		36. 391	1.00 13.23	A	Ċ
ATOM	3166	CD2	TYR	417	28. 071	64.622	33. 718	1.00 17.72	A	С
ATOM ATOM	3167 3168	CEZ	TYR TYR	417 417	27. 120 27. 488		34. 710 36. 040	1.00 15.27 1.00 14.25	A A	C C
ATOM	3169	OH	TYR	417	26. 556	65.046	37.020	1.00 14.06	Α	0
ATOM	3170	C	TYR	417	30. 768		33. 747	1.00 18.77 1.00 18.74	A A	C 0
ATOM ATOM	3171 3172	0 N	TYR ILE	417 418	29. 918 31. 996		34. 207 34. 236	1.00 18.74	A	N N
ATOM	3173	CA	ILE	418	32. 429	60.926	35. 379	1.00 16.60	Α	С
ATOM	3174	CB	ILE	418	33. 626		35. 015	1.00 15.54 1.00 14.33	A A	C
ATOM ATOM	3175 3176		ILE ILE	418 418	34. 482 33. 107		36. 241 34. 378	1.00 14.33	A	C C C
ATOM	3177	CD1	ILE	418	34. 183	57.767	33.964	1.00 15.48	Α	Ċ
ATOM	3178	C	ILE	418	32. 827		36. 453	1.00 18.54	A	C 0
ATOM ATOM	3179 3180	O N	ILE SER	418 419	33. 535 32. 356		36. 190 37. 664	1.00 20.83 1.00 19.59	A A	N
ATOM	3181	CA	SER	419	32.670	62.556	38.764	1.00 20.34	Α	C
ATOM	3182	CB	SER	419	31. 523		38. 996	1.00 21.79	A	C
ATOM ATOM	3183 3184	OG C	SER SER	419 419	30. 415 32. 875		39. 562 40. 013	1. 00 24. 33 1. 00 20. 37	A A	0 C

										(Cont	inued)
					FΙ	G. 4	- 66				
ATOM ATOM ATOM	3185 3186 3187	O N CA	SER ASN ASN	419 420 420	32. 783 33. 152 33. 357	60. 503 62. 427 61. 786	39. 988 41. 107 42. 387	1.00 20.32 1.00 19.64 1.00 20.07	A A A	0 N C	
ATOM ATOM	3188 3189	CB CG	ASN ASN	420 420	34. 773 35. 099	62. 053 63. 518	42. 863 42. 872	1.00 18.49 1.00 20.69	A A	C	
ATOM ATOM	3190 3191	OD1 ND2	ASN	420 420	34. 210 36. 376	64. 358 63. 844	42. 741 43. 034	1.00 21.49 1.00 21.39	A A	O N	
ATOM ATOM	3192 3193	C 0	ASN ASN	420 420	32. 350 32. 677	62. 368 62. 610	43. 379 44. 535	1.00 20.90 1.00 21.17	A A	C 0	
ATOM ATOM	3194 3195	N CA	GLU GLU	421 421	31.127 30.081	62. 600 63. 160	42. 914 43. 761	1.00 21.68 1.00 24.26	A A	N C	
ATOM ATOM	3196 3197	CB CG	GLU GLU	421 421	28. 935 27. 714	63. 722 64. 214	42. 901 43. 701	1.00 26.18 1.00 25.32	A A	C C	
ATOM ATOM	3198 3199		GLU GLU	421 421	26. 604 25. 563	64. 817 65. 237 64. 873	42. 824 43. 373 41. 588	1.00 26.09 1.00 24.11 1.00 27.22	A A A	C 0 0	
ATOM ATOM ATOM	3200 3201 3202	0E2 C 0	GLU GLU GLU	421 421 421	26. 762 29. 512 29. 185	62. 133 62. 457	44. 729 45. 868	1.00 24.93 1.00 27.30	A A	C O	
ATOM ATOM	3203 3204	N CA	TYR TYR	422 422	29. 409 28. 837	60. 892 59. 826	44. 272 45. 075	1.00 23.63 1.00 23.67	A A	N C	
ATOM ATOM	3205 3206	CB CG	TYR TYR	422 422	28. 942 28. 015	58. 503 57. 415	44. 311 44. 813	1.00 23.61 1.00 24.39	A A	C C	
ATOM ATOM	3207 3208	CE1	TYR TYR	422 422	26. 642 25. 781	57. 637 56. 618	44. 936 45. 347	1.00 23.87 1.00 22.11	A A	C C	
ATOM ATOM	3209 3210	CE2	TYR TYR	422 422	28.505 27.654	56. 147 55. 124	45. 120 45. 533	1.00 24.53 1.00 23.32	A A	C	
ATOM ATOM	3211 3212	CZ OH	TYR TYR	422 422	26. 300 25. 471	55. 367 54. 349	45. 641 46. 031	1.00 23.52 1.00 24.33	A A	C 0 C	
ATOM ATOM	3213 3214 3215	C O N	TYR TYR LYS	422 422 423	29. 399 30. 599 28. 492	59. 679 59. 478 59. 784	46. 493 46. 704 47. 461	1.00 23.57 1.00 23.17 1.00 23.07	A A A	O N	
ATOM ATOM ATOM	3216 3217	CA CB	LYS LYS	423 423 423	28. 813 29. 156	59. 661 58. 205	48. 878 49. 205	1.00 23.01 1.00 22.04 1.00 24.22	A A	C C	
ATOM ATOM	3218 3219	CG CD	LYS LYS	423 423	27. 967 28. 303	57. 266 55. 809	49.009 49.276	1.00 25.11 1.00 26.55	A A	Č C	
ATOM ATOM	3220 3221	CE NZ	LYS LYS	423 423	27. 079 27. 302	54. 930 53. 498	49. 002 49. 336	1.00 28.11 1.00 27.79	A A	C N	
ATOM ATOM	3222 3223	C 0	LYS LYS	423 423	29. 923 30. 533	60. 583 60. 340	49. 347 50. 385	1.00 21.46 1.00 20.97	A A	C 0	
ATOM ATOM	3224 3225	N CA	GLY GLY	424 424	30.167 31.201	61. 647 62. 608	48. 583 48. 930	1.00 21.39	A A	N C	
ATOM ATOM ATOM	3226 3227 3228	C O N	GLY GLY MET	424 424 425	32.606 33.463 32.848	62. 034 62. 534 60. 991	48. 961 49. 687 48. 173	1.00 21.98 1.00 22.19 1.00 22.44	A A A	C O N	
ATOM ATOM	3229 3230	CA CB	MET MET	425 425 425	34.161 34.003	60. 350 58. 826	48. 134 48. 056	1.00 23.29 1.00 24.14	A A	C C	
ATOM ATOM	3231 3232	CG SD	MET MET	425 425	33. 548 33. 092	58. 187 56. 451	49.360 49.179	1.00 25.32 1.00 29.39	A A	C S	
ATOM	3233	CE	MET	425	34.663	55. 611	49. 406	1.00 27.92	A	С	

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				FIG. 4-67	(Continued)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	3234 3235 3236 3237 3238 3240 3241 3242 3243 3244 3245 3246 3247 3248 3249 3250 3251 3252 3253 3254 3255	O MET N PRO CD PRO CA PRO CB PRO C PRO O PRO N GLY CA GLY O GLY N GLY CA GLY O GLY N ARG CA ARG CA ARG CB ARG CC ARG CD ARG	425 426 426 426 426 426 426 427 427 427 427 427 428 428 428 429 429 429 429	35. 042 60. 827 46. 986 1. 00 22. 06 34. 836 60. 457 45. 835 1. 00 22. 61 36. 045 61. 661 47. 292 1. 00 21. 75 36. 386 62. 215 48. 615 1. 00 21. 34 36. 951 62. 172 46. 262 1. 00 20. 07 37. 943 63. 007 47. 062 1. 00 20. 22 37. 138 63. 461 48. 245 1. 00 19. 61 37. 636 61. 019 45. 532 1. 00 20. 63 37. 920 61. 107 44. 343 1. 00 23. 99 37. 905 59. 936 46. 252 1. 00 19. 08 38. 552 58. 789 45. 646 1. 00 18. 03 37. 601 57. 838 44. 941 1. 00 18. 93 37. 965 56. 706 44. 642 1. 00 21. 55 36. 378 58. 285 44. 684 1. 00 18. 22 35. 417 57. 446 43. 991 1. 00 17. 96 35. 208 57. 970 42. 583 1. 00 19. 00 34. 619 57. 158 41. 712 1. 00 16. 78 34. 389 57. 559 40. 320 1. 00 17. 38 35. 595 57. 167 39. 444 1. 00 19. 09 36. 577 58. 292 39. 108 1. 00 20. 57 37. 385 58. 737 40. 302 1. 00 22. 65	(Continued) A C A O A N A C A C A C A C A C A C A C A C A C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	3256 3257 3258 3259 3260 3261 3262 3263 3264 3265 3266	NE ARG CZ ARG NH1 ARG NH2 ARG C ARG O ARG N ASN CA ASN CB ASN CG ASN OD1 ASN	429 429 429 429 429 430 430 430 430 430	38. 359 59. 769 39. 956 1. 00 25. 75 39. 078 60. 445 40. 852 1. 00 26. 83 38. 927 60. 204 42. 146 1. 00 26. 78 39. 957 61. 356 40. 456 1. 00 26. 24 33. 134 56. 889 39. 756 1. 00 15. 74 32. 976 55. 675 39. 857 1. 00 12. 14 32. 256 57. 679 39. 146 1. 00 14. 98 31. 027 57. 136 38. 586 1. 00 17. 41 29. 901 57. 216 39. 622 1. 00 17. 29 29. 947 56. 081 40. 620 1. 00 18. 53 29. 607 54. 938 40. 297 1. 00 16. 68	A C A N A C A O C A C A C A C A C A C A C A C A
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	3267 3268 3269 3270 3271 3272 3273 3274 3275 3276 3277 3278 3279 3280 3281 3282	ND2 ASN C ASN N LEU CA LEU CG LEU CD1 LEU CD2 LEU C LEU O LEU N TYR CA TYR CB TYR CG TYR CGT TYR	430 430 431 431 431 431 431 431 431 432 432 432 432	30. 381 56. 386 41. 840 1. 00 15. 65 30. 564 57. 808 37. 297 1. 00 17. 98 30. 849 58. 976 37. 043 1. 00 19. 64 29. 840 57. 053 36. 485 1. 00 17. 00 29. 314 57. 576 35. 241 1. 00 17. 70 29. 122 56. 442 34. 231 1. 00 15. 35 28. 478 56. 867 32. 913 1. 00 15. 33 29. 340 57. 917 32. 230 1. 00 13. 77 28. 296 55. 645 32. 018 1. 00 17. 37 27. 978 58. 279 35. 491 1. 00 19. 03 27. 095 57. 750 36. 172 1. 00 17. 62 27. 840 59. 475 34. 933 1. 00 20. 33 26. 620 60. 248 35. 083 1. 00 21. 23 26. 848 61. 442 36. 014 1. 00 22. 85 27. 068 61. 070 37. 464 1. 00 25. 34 28. 320 60. 646 37.	A N A C A C A C A C A C A C A C A C A C

					(Continued)
				FIG. 4-68	(Oontinued)
A TOM	0000	CD1 TVD	499	28.519 60.305 39.267 1.00 24.97 A	C
ATOM	3283 3284	CE1 TYR CD2 TYR	432 432	28. 519 60. 305 39. 267 1. 00 24. 97 A 26. 019 61. 142 38. 384 1. 00 24. 85 A	C C
ATOM ATOM	3285	CE2 TYR	432	26. 205 60. 805 39. 723 1. 00 25. 31 A	Č
ATOM	3286	CZ TYR	432	27. 454 60. 388 40. 161 1. 00 25. 88 A	č
ATOM	3287	OH TYR	432	27. 625 60. 054 41. 487 1. 00 25. 59 A	ŏ
ATOM	3288	C TYR	432	26. 102 60. 743 33. 737 1. 00 21. 26 A	č
ATOM	3289	0 TYR	432	26. 860 60. 870 32. 770 1. 00 21. 07 A	Ŏ
ATOM	3290	N LYS	433	24.802 61.022 33.695 1.00 20.78 · A	N
ATOM	3291	CA LYS	433	24. 133 61. 505 32. 496 1. 00 20. 98 A	C
ATOM	3292	CB LYS	433	23. 290 60. 386 31. 876 1. 00 21. 14 A	C
ATOM	3293	CG LYS	433	22. 564 60. 827 30. 618 1. 00 25. 64 A	C
ATOM	3294	CD LYS	433	21. 843 59. 701 29. 907 1. 00 25. 30 A	C
ATOM	3295	CE LYS	433	20. 643 59. 235 30. 682 1. 00 25. 25 A	C
ATOM	3296	NZ LYS	433	19.801 58.370 29.817 1.00 27.99 A	N
ATOM	3297	C LYS	433	23. 228 62. 687 32. 835 1. 00 20. 46 A	C
ATOM	3298	0 LYS	433	22. 367 62. 587 33. 707 1. 00 21. 41 A	0
ATOM	3299	N ILE	434	23. 427 63. 812 32. 162 1. 00 20. 15 A	N
ATOM	3300	CA ILE	434	22. 591 64. 980 32. 417 1. 00 21. 18 A	C
ATOM	3301	CB ILE	434	23. 427 66. 225 32. 815 1. 00 21. 51 A	C
ATOM	3302	CG2 ILE	434	24. 412 66. 582 31. 715 1. 00 22. 39 A	C
ATOM	3303	CG1 ILE	434	22.491 67.404 33.083 1.00 22.04 A	C
ATOM	3304	CD1 ILE	434	23.171 68.591 33.699 1.00 23.38 A	C
ATOM ATOM	3305 3306	C ILE 0 ILE	434 434	21. 782 65. 297 31. 174 1. 00 20. 81 A 22. 274 65. 154 30. 056 1. 00 21. 15 A	C 0
ATOM	3307	N GLN	434	22. 274 65. 154 30. 056 1. 00 21. 15 A 20. 538 65. 716 31. 372 1. 00 21. 40 A	N N
ATOM	3308	CA GLN	435	19.666 66.034 30.248 1.00 23.73 A	C
ATOM	3309	CA GLN	435	18. 202 65. 851 30. 646 1. 00 26. 08 A	Č
ATOM	3310	CG GLN	435	17. 227 66. 030 29. 496 1. 00 29. 99 A	č
ATOM	3311	CD GLN	435	15. 802 65. 806 29. 929 1. 00 32. 10 A	č
ATOM	3312	OE1 GLN	435	15. 446 64. 720 30. 372 1. 00 34. 41 A	ŏ
ATOM	3313	NE2 GLN	435	14. 978 66. 839 29. 819 1. 00 34. 05 A	Ň
ATOM	3314	C GLN	435	19.891 67.450 29.743 1.00 22.81 A	Ċ
ATOM	3315	O GLN	435	19.600 68.419 30.434 1.00 22.20 A	Ō
ATOM	3316	N LEU	436	20. 401 67. 564 28. 524 1. 00 23. 57 A	N
ATOM	3317	CA LEU	436	20. 679 68. 865 27. 951 1. 00 24. 55 A	С
ATOM	3318	CB LEU	436	21. 152 68. 714 26. 508 1. 00 21. 18 A	С
ATOM	3319	CG LEU	436	22. 456 67. 939 26. 332 1. 00 21. 36 A	С
ATOM	3320	CD1 LEU	436	22.938 68.116 24.910 1.00 20.02 A	C
ATOM	3321	CD2 LEU	436	23.510 68.437 27.317 1.00 19.70 A	С
ATOM	3322	C LEU	436	19. 491 69. 812 28. 020 1. 00 26. 85 A	C
ATOM	3323	0 LEU	436	19. 672 71. 016 28. 168 1. 00 28. 66 A	0
ATOM	3324	N SER	437	18. 280 69. 268 27. 927 1. 00 30. 22 A	N
ATOM	3325	CA SER	437	17. 059 70. 075 27. 977 1. 00 32. 38 A	C
ATOM	3326	CB SER	437	15. 925 69. 340 27. 268 1. 00 32. 98 A	C
ATOM	3327	OG SER	437	16. 241 69. 151 25. 901 1. 00 39. 22 A	0
ATOM	3328 3329	C SER	437	16.610 70.437 29.394 1.00 33.81 A	C
ATOM	3330	O SER N ASP	437 438	15. 805 71. 352 29. 577 1. 00 32. 20 A 17. 124 69. 714 30. 387 1. 00 35. 36 A	0
ATOM ATOM	3331	CA ASP	438 438	17. 124 69. 714 30. 387 1. 00 35. 36 A 16. 772 69. 955 31. 784 1. 00 36. 00 A	N C
WIOIT	0001	on noi	400	10.112 UJ. JUU UI. 104 1. UU UU. UU M	U

				FIG. 4-70	(Continue	d)
		04 0770	444		С	
ATOM	3381	CA CYS	444		Č	
ATOM	3382	C CYS	444	23. 758 56. 712 37. 157 1. 00 22. 91 A 22. 855 55. 990 37. 573 1. 00 21. 72 A	Ö	
ATOM	3383	O CYS CB CYS	444 444	24. 396 58. 018 39. 219 1. 00 25. 50 A	č	
ATOM	3384 3385	CB CYS	444	26. 053 57. 282 39. 443 1. 00 30. 81 A	Š	
ATOM ATOM	3386	N LEU	445	24. 573 56. 348 36. 175 1. 00 22. 64 A	N	
ATOM	3387	CA LEU	445	24. 446 55. 053 35. 513 1. 00 22. 51 A	C	
ATOM	3388	CB LEU	445	24. 799 55. 211 34. 035 1. 00 19. 29 A	С	
ATOM	3389	CG LEU	445	24. 049 56. 349 33. 341 1. 00 19. 36 A	C	
ATOM	3390	CD1 LEU	445	24.588 56.552 31.934 1.00 16.01 A	C	
ATOM	3391	CD2 LEU	445	22. 559 56. 034 33. 319 1. 00 15. 72 A	C	
ATOM	3392	C LEU	445	25. 308 53. 940 36. 118 1. 00 23. 32 A	C	
ATOM	3393	0 LEU	445	25. 203 52. 783 35. 718 1. 00 24. 58 A	0	
ATOM	3394	N SER	446	26. 148 54. 274 37. 087 1. 00 23. 95 A	N C	
ATOM	3395	CA SER	446	27. 028 53. 269 37. 660 1. 00 23. 89 A	C	
ATOM	3396	CB SER	446	28. 469 53. 555 37. 222 1. 00 21. 87 A 28. 882 54. 847 37. 648 1. 00 20. 09 A	Ö	
ATOM	3397	OG SER C SER	446 446	28. 882 54. 847 37. 648 1. 00 20. 09 A 26. 969 53. 145 39. 175 1. 00 23. 77 A	Č	
ATOM ATOM	3398 3399	C SER O SER	446 446	27. 361 52. 119 39. 720 1. 00 24. 69 A	ŏ	
ATOM	3400	N CYS	447	26. 480 54. 184 39. 845 1. 00 24. 32 A	N	
ATOM	3401	CA CYS	447	26. 382 54. 207 41. 309 1. 00 26. 45 A	С	
ATOM	3402	C CYS	447	25.836 52.946 41.997 1.00 25.99 A	C	
ATOM	3403	0 CYS	447	26. 441 52. 425 42. 937 1. 00 24. 44 A	Ō	
ATOM	3404	CB CYS	447	25. 518 55. 396 41. 763 1. 00 27. 33 A	C	
ATOM	3405	SG CYS	447	26. 225 57. 049 41. 461 1. 00 34. 75 A	S	
ATOM	3406	N GLU	448	24. 696 52. 456 41. 528 1. 00 25. 90 A		
ATOM	3407	CA GLU	448	24. 056 51. 317 42. 167 1. 00 24. 38 A 22. 581 51. 637 42. 334 1. 00 23. 47 A		
ATOM	3408	CB GLU CG GLU	448 448	22. 581 51. 637 42. 334 1. 00 23. 47 A 22. 332 53. 075 42. 721 1. 00 24. 60 A		
ATOM ATOM	3409 3410	CG GLU	448	22. 848 53. 416 44. 108 1. 00 27. 44 A	and the second s	
ATOM	3411	OE1 GLU	448	22.617 54.562 44.559 1.00 29.17 A	•	
ATOM	3412	OE2 GLU	448	23. 478 52. 548 44. 751 1. 00 28. 81 A	0	
ATOM	3413	C GLU	448	24. 201 49. 941 41. 537 1. 00 23. 54 A		
ATOM	3414	0 GLU	448	23. 722 48. 970 42. 104 1. 00 22. 25 A		
ATOM	3415	n leu	449	24. 844 49. 844 40. 377 1. 00 23. 78 A		
ATOM	3416	CA LEU	449	25. 024 48. 547 39. 717 1. 00 23. 34 A		
ATOM	3417		449			
ATOM	3418	CG LEU	449	25. 680 49. 712 37. 472 1. 00 21. 20 A 26. 872 49. 807 36. 543 1. 00 20. 05 A	_	
ATOM	3419	CD1 LEU	449	26. 872 49. 807 36. 543 1. 00 20. 05 A 24. 424 49. 335 36. 711 1. 00 17. 29 A	_	
ATOM	3420 3421	CD2 LEU C LEU	449 449	25. 551 47. 456 40. 654 1. 00 24. 61 A		
ATOM ATOM	3422	0 LEU	449	25. 157 46. 298 40. 549 1. 00 26. 01 A		
ATOM	3423	N ASN	450	26. 445 47. 830 41. 562 1. 00 25. 89 A		
ATOM	3424	CA ASN	450	27. 040 46. 889 42. 512 1. 00 27. 02 A		
ATOM	3425	CB ASN	450	27. 939 45. 913 41. 754 1. 00 27. 92 A		
ATOM	3426	CG ASN	450	28. 296 44. 695 42. 572 1. 00 31. 61 A		
ATOM	3427	OD1 ASN	450	28. 521 44. 786 43. 783 1. 00 34. 65 A		
ATOM	3428		450	28. 363 43. 541 41. 912 1. 00 31. 27 A	_	
ATOM	3429	C ASN	450	27. 877 47. 731 43. 488 1. 00 26. 54 A	·	

				FIG. 4-71	(Continued)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	3430 3431 3432 3433 3434 3435 3436 3441 3442 3443 3444 3445 3446 3447 3450 3451 3452 3453 3454 3455 3456 3457 3458 3459 3460 3461 3462	O ASN N PRO CD PRO CA PRO CB PRO C PRO O PRO N GLU CB GLU CB GLU OE2 GLU OE2 GLU N ARG CA ARG CB ARG CC ARG CB ARG CC ARG NE ARG CC ARG NE ARG CC ARG NE ARG CC ARG NE ARG CC CYS CC CYS CC CYS CC CYS	451 451 451 451 452 452 452 452 452 453 453 453 453 453 454 454 454 454 454	FIG. 4 - 71 29. 099 47. 637 43. 523 1. 00 26. 25 27. 210 48. 558 44. 303 1. 00 27. 04 25. 762 48. 411 44. 535 1. 00 27. 72 27. 796 49. 465 45. 296 1. 00 27. 49 26. 579 49. 924 46. 103 1. 00 27. 21 25. 638 48. 765 45. 989 1. 00 25. 73 28. 938 48. 983 46. 187 1. 00 28. 75 29. 877 49. 737 46. 433 1. 00 30. 69 28. 873 47. 746 46. 666 1. 00 29. 54 29. 918 47. 228 47. 545 1. 00 30. 30 29. 453 45. 937 48. 232 1. 00 33. 99 28. 085 46. 024 48. 890 1. 00 39. 92 27. 817 44. 848 49. 813 1. 00 45. 87 28. 084 43. 693 49. 402 1. 00 47. 97 27. 336 45. 076 50. 948 1. 00 47. 68 31. 221 46. 946 46. 816 1. 00 29. 63 32. 308 47. 199 47. 344 1. 00 30. 27 31. 099 46. 425 45. 600 1. 00 27. 01 32. 244 46. 057 44. 783 1. 00 24. 90 31. 950 44. 728 44. 085 1. 00 23. 08 32. 308 47. 199 47. 344 1. 00 30. 27 31. 999 46. 425 45. 600 1. 00 27. 01 32. 244 46. 057 44. 783 1. 00 24. 90 31. 950 44. 728 44. 085 1. 00 23. 08 32. 308 47. 199 47. 344 1. 00 30. 27 31. 099 46. 425 45. 600 1. 00 27. 01 32. 244 46. 057 44. 783 1. 00 24. 90 33. 504 42. 688 41. 278 1. 00 18. 31 33. 439 41. 595 40. 531 1. 00 18. 93 33. 504 42. 688 41. 278 1. 00 18. 31 33. 439 41. 595 40. 531 1. 00 18. 93 32. 510 40. 679 40. 763 1. 00 19. 77 34. 302 41. 425 39. 539 1. 00 18. 87 34. 302 41. 425 39. 539 1. 00 18. 87 32. 695 47. 071 43. 738 1. 00 25. 72 33. 809 46. 962 43. 222 1. 00 24. 32 31. 857 48. 054 43. 420 1. 00 25. 94 32. 233 49. 012 42. 385 1. 00 25. 49 32. 038 50. 473 42. 699 1. 00 24. 24 30. 922 50. 970 42. 688 1. 00 26. 79 31. 503 48. 664 41. 096 1. 00 26. 13	
ATOM ATOM ATOM	3463 3464 3465	SG CYS N GLN CA GLN	454 455 455	32. 156 47. 128 40. 401 1. 00 30. 12 A 33. 143 51. 165 42. 942 1. 00 22. 97 A 33. 105 52. 576 43. 276 1. 00 23. 69 A	C S N C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM	3466 3467 3468 3469 3470 3471 3472	CB GLN CG GLN CD GLN OE1 GLN NE2 GLN C GLN O GLN	455 455 455 455 455 455 455	33. 536 52. 761 44. 736 1. 00 23. 41 A 32. 564 52. 187 45. 761 1. 00 24. 96 A 33. 177 52. 065 47. 150 1. 00 29. 34 A 33. 981 52. 907 47. 574 1. 00 30. 98 A 32. 790 51. 022 47. 872 1. 00 28. 59 A 33. 992 53. 425 42. 360 1. 00 24. 57 A 33. 837 54. 645 42. 294 1. 00 27. 40	C C O N C
ATOM ATOM ATOM ATOM ATOM ATOM	3473 3474 3475 3476 3477 3478	N TYR CA TYR CB TYR CG TYR CD1 TYR CE1 TYR	456 456 456 456 456 456	34. 919 52. 787 41. 654 1. 00 22. 57 A 35. 821 53. 510 40. 763 1. 00 21. 75 A 37. 270 53. 187 41. 124 1. 00 20. 47 A 38. 267 54. 282 40. 817 1. 00 21. 27 A 38. 659 55. 193 41. 808 1. 00 20. 27 A 39. 618 56. 165 41. 548 1. 00 18. 67 A	N C C C C C

					FΙ	G. 4	- 72			(Contin	nued
ATOM	3479		TYR	456	38. 858	54. 385	39. 552	1.00 19.29	Α	C	
ATOM	3480		TYR	456	39.812	55. 353	39. 284	1.00 16.18	Α	C	
ATOM	3481	CZ	TYR	456	40. 190	56. 236	40. 283	1.00 18.92	Α	C	
ATOM	3482	OH	TYR	456	41.151	57. 183	40.023	1.00 19.64	Α	0	
ATOM	3483	C	TYR	456	35. 536	53.061	39. 335	1.00 21.96	Α	C	
ATOM	3484	0	TYR	456	35. 944	51.972	38. 931	1.00 22.39	Α	0	
ATOM	3485	N	TYR	457	34.846	53. 899	38. 567	1.00 22.09	A	N.	
ATOM	3486	CA	TYR	457	34.499	53.540	37. 196	1.00 20.82	Α	C	
ATOM	3487	CB	TYR	457	33. 001	53. 717	36.956	1.00 17.91	A	C	
ATOM	3488	CG	TYR	457	32. 147	52. 613	37.512	1.00 15.58	A	C	
ATOM	3489		TYR	457	31.644	52.674	38. 811	1.00 13.21	A	C	
ATOM	3490		TYR	457	30. 830	51.668	39. 311	1.00 12.43	A	C	
ATOM	3491		TYR	457	31.819	51.512	36. 727	1.00 16.86	A	C	
ATOM	3492		TYR	457	31.008	50. 497	37. 219	1.00 15.29	A	C	
ATOM	3493	CZ	TYR	457	30.518	50. 582	38. 507	1.00 14.49	A	C	
ATOM	3494	OH C	TYR	457	29. 728	49. 568	38.985	1.00 15.62	A	0	
ATOM	3495	C	TYR	457	35. 232	54. 240	36.066 36.227	1.00 21.27	A	C	
ATOM	3496	O N	TYR SER	457 458	35. 842 35. 132	55. 293 53. 622	34. 901	1.00 23.18 1.00 21.68	A	O N	
ATOM ATOM	3497 3498	ÇA	SER	458	35. 739	54. 108	33. 683	1.00 21.08	A	C	
ATOM	3499	CB	SER	458 458	37. 083	53. 429	33. 474	1.00 21.74	A	C	
ATOM	3500	OG	SER	4=0	05 510	53. 569	32. 141	1.00 29.63	A A	Õ	
ATOM	3501	C	SER	458 . 458	34. 751	53. 664	32. 621	1.00 23.03	A	C	
ATOM	3502	0	SER	458	34. 072	52. 652	32. 804	1.00 20.08	A	Ö	
ATOM	3503	N	VAL	459	34.665	54. 405	31.520	1.00 20.58	A	N	
ATOM	3504	CA	VAL	459	33. 722	54.061	30.468	1.00 19.99	A	Ĉ	
ATOM	3505	CB	VAL	459	32. 457	54. 949	30. 568	1.00 19.45	Ä	č	
ATOM	3506		VAL	459	32. 816	56. 392	30. 308	1.00 19.10	Ä	č	
ATOM	3507		VAL	459	31. 397	54. 475	29. 595	1.00 20.30	A	Č	
ATOM	3508	C	VAL	459	34. 309	54. 161	29.059	1.00 19.99	Ā	Č	
ATOM	3509	0	VAL	459	35. 314	54.835	28.831	1.00 21.13	A	0	
ATOM	3510	N	SER	460	33.667	53.472	28.122	1.00 18.73	Α	N	
ATOM	3511	CA	SER	460	34.083	53. 456	26.728	1.00 16.25	Α	C	
ATOM	3512	CB	SER	460	34.970	52.230	26.476	1.00 16.33	Α	C	
ATOM	3513	0G	SER	460	35.476	52.194	25.151	1.00 15.85	Α	0	
ATOM	3514	C	SER	460	32.809	53. 377	25.883	1.00 15.70	Α	C	
ATOM	3515	0		460	32. 156	52. 342		1.00 14.81	Α	0	
ATOM	3516	N	PHE	461	32.450	54. 475	25.226	1.00 16.00	Α	N	
ATOM	3517	CA	PHE	461	31.245	54. 512	24.398	1.00 16.27	Α	C	
ATOM	3518	CB	PHE	461	30. 636	55. 921	24. 367	1.00 15.50	A	С	
ATOM	3519		PHE	461	30.001	56. 351	25.660	1.00 15.11	A	C	
ATOM	3520		PHE	461	30. 779	56. 764	26.735	1.00 14.16	Ą	C	
ATOM	3521		PHE	461	28.617	56.340	25.804	1.00 14.86	A	C	
ATOM	3522		PHE	461	30. 190	57. 158	27. 931	1.00 12.94	A	C	
ATOM	3523		PHE	461	28. 021	56. 733	26. 996	1.00 12.76	A	C	
ATOM	3524	CZ	PHE	461	28. 811	57. 142	28.061	1.00 11.01	A	C	
ATOM	3525	C	PHE	461	31.551	54. 102	22.971	1.00 17.94	A	C	
ATOM	3526	0 N	PHE	461	32.686	54. 234	22.514	1.00 17.07	A	0 N	
ATOM	3527	N	SER	462	30. 532	53.612	22.269	1.00 19.22	Α	N	

					FΙ	G. 4	- 73			(Continued)
ATOM ATOM ATOM ATOM ATOM	3528 3529 3530 3531 3532 3533	CB OG C O	SER 4 SER 4 SER 4 SER 4 LYS 4	62 62 62 62 62 63	30. 694 29. 494 28. 308 30. 804 30. 572 31. 153	53. 212 52. 381 53. 145 54. 496 55. 581 54. 373	20. 877 20. 399 20. 397 20. 058 20. 577 18. 784	1.00 23.70 1.00 23.50 1.00 24.06 1.00 24.95 1.00 25.95 1.00 27.50	A A A A	C C O C O N
ATOM ATOM ATOM ATOM ATOM ATOM ATOM	3534 3535 3536 3537 3538 3539 3540	CB I CG I CD I CE I NZ I	LYS 4 LYS 4 LYS 4 LYS 4 LYS 4	63 63 63 63 63 63	31. 323 31. 587 33. 047 33. 972 35. 433 36. 384 30. 226	55. 536 55. 084 55. 199 54. 435 54. 724 54. 098 56. 602	17. 920 16. 484 16. 075 17. 007 16. 673 17. 641 17. 934	1.00 31.80 1.00 33.43 1.00 35.54 1.00 36.78 1.00 39.20 1.00 40.26 1.00 33.39	A A A A A	C C C C C N
ATOM ATOM ATOM ATOM ATOM ATOM ATOM	3541 3542 3543 3544 3545 3546 3547	N (CA (CB (CG	GLU 4 GLU 4 GLU 4 GLU 4 GLU 4	63 64 64 64 64 64	30. 484 29. 015 27. 945 26. 960 27. 528 26. 578 25. 439	57. 745 56. 254 57. 247 57. 058 57. 366 56. 961 57. 480	17. 561 18. 354 18. 410 17. 256 15. 882 14. 772 14. 752	1.00 36.36 1.00 33.23 1.00 34.54 1.00 39.82 1.00 44.96 1.00 48.72 1.00 50.39	A A A A A	O N C C C C O
ATOM ATOM ATOM ATOM ATOM ATOM ATOM	3548 3549 3550 3551 3552 3553 3554	OE2 C C C O C N A CA A CB A	GLU 4 GLU 4 GLU 4 ALA 4 ALA 4 ALA 4 ALA 4	64 64 64 65 65 65	26. 967 27. 186 26. 047 27. 823 27. 241 26. 889 26. 015	56. 120 57. 202 57. 659 56. 636 56. 546 57. 935	13. 926 19. 729 19. 814 20. 748 22. 081 22. 577	1.00 50.59 1.00 32.77 1.00 32.03 1.00 31.17 1.00 29.63 1.00 28.36	A A A A	O C O N C C
ATOM ATOM ATOM ATOM ATOM ATOM	3555 3556 3557 3558 3559 3560	O A I CA L CB L CC L CD L	ALA 4 LYS 4 LYS 4 LYS 4 LYS 4 LYS 4	65 66 66 66 66	25. 176 25. 905 24. 763 24. 585 23. 208 23. 045	55. 645 55. 824 54. 678 53. 772 53. 122 52. 509 52. 179	22. 164 23. 042 21. 259 21. 274 19. 899 19. 649 18. 171	1.00 29.47 1.00 28.66 1.00 28.89 1.00 28.97 1.00 30.98 1.00 31.77 1.00 34.52	A A A A A	C O N C C C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM	3561 3562 3563 3564 3565 3566 3567	NZ L C L O L N T CA T	.YS 4 .YS 4 .YS 4 .YR 4 .YR 4	56 56 56 57 57	21. 632 21. 273 24. 987 24. 040 26. 252 26. 599 26. 955	51. 757 50. 441 52. 704 52. 126 52. 446 51. 458 50. 119	17. 814 18. 404 22. 339 22. 869 22. 646 23. 654 23. 003	1. 00 35. 82 1. 00 38. 42 1. 00 28. 20 1. 00 27. 93 1. 00 26. 93 1. 00 26. 21 1. 00 27. 94	A A A A A	C N C O N C C
ATOM ATOM ATOM ATOM ATOM ATOM	3568 3569 3570 3571 3572 3573	CG T CD1 T CE1 T CD2 T CE2 T CZ T	YR 40 YR 40 YR 40 YR 40 YR 40 YR 40	57 57 57 57 57	25. 823 25. 550 24. 494 25. 009 23. 953 23. 698	49. 502 49. 917 49. 373 48. 522 47. 975 48. 405	22. 207 20. 903 20. 184 22. 768 22. 060 20. 770	1.00 21.34 1.00 30.39 1.00 29.93 1.00 31.13 1.00 29.73 1.00 30.29 1.00 30.97	A A A A A	C C C C C
ATOM ATOM ATOM	3574 3575 3576	C T	YR 46 YR 46 YR 46	7	22. 625 27. 777 28. 491	47. 890 51. 949 52. 852	20. 079 24. 470 24. 064	1.00 32.01 1.00 24.00 1.00 24.63	. A . A . A	0 C 0

				F]	G. 4	- 74			(Continued)
ATOM	3577	N T	YR 468	27. 969	51.370	25.641	1.00 23.06	A	N
ATOM	3578	CA T	YR 468	29. 091	51.765	26.462	1.00 22.80	A	С
ATOM	3579	CB T	YR 468			27. 249	1.00 23.88	Α	С
ATOM	3580		YR 468			28. 155	1.00 24.49	A	C
ATOM	3581	CD1 T				27.646	1.00 23.81	A	C
ATOM	3582	CE1 T			53.308	28. 486	1.00 25.51	A	C
ATOM	3583	CD2 T				29. 537	1.00 26.39	A	C
ATOM	3584	CE2 T			52.971	30. 390	1.00 25.67	A	C
ATOM	3585		YR 468			29.857	1.00 25.81	A	C
ATOM	3586		YR 468			30. 695	1.00 25.95	A	0 .
ATOM	3587		YR 468			27.411	1.00 21.32	A	C 0
ATOM	3588		YR 468			28. 070 27. 449	1.00 22.73 1.00 20.26	A A	. N
ATOM	3589		LN 469 LN 469			28.315	1.00 20.20	A	C
ATOM ATOM	3590 3591		LN 469 LN 469			27. 695	1.00 19.21	A	. C
ATOM	3592		LN 469			28. 632	1.00 20.12	A	Č
ATOM	3593		LN 469			28. 169	1.00 23.85	A	č
ATOM	3594	0E1 G				28. 011	1.00 25.81	A	ŏ
ATOM	3595	NE2 G				27. 948	1.00 23.84	Ä	Ň
ATOM	3596		LN 469			29. 589	1.00 19.50	Ä	Ĉ
ATOM	3597		LN 469			29. 549	1.00 19.63	Ā	0
ATOM	3598		EU 470			30.716	1.00 19.27	A	N
ATOM	3599		EU 470			32.002	1.00 20.27	Α	C
ATOM	3600		EU 470		50.136	32.961	1.00 20.14	Α	C
ATOM	3601	CG L	EU 470		2 51.323	32.929	1.00 21.50	Α	C
ATOM	3602	CD1 L	EU 470			33.996	1.00 19.33	Α	C
ATOM	3603	CD2 L				33. 184	1.00 19.44	Α	С
ATOM	3604		EU 470			32. 531	1.00 20.91	A	C
ATOM	3605		.EU 470			32.409	1.00 19.97	A	0
ATOM	3606		RG 471	33. 753	3 50.050	33. 102	1.00 22.57	A	Ŋ
ATOM	3607		RG 471	34. 917	49.344	33.610	1.00 25.83	A	C
ATOM	3608		RG 471			32.748	1.00 29.78	A	C
ATOM	3609		RG 471			31.261	1.00 31.73	A	C
ATOM	3610		IRG 471			30. 426	1.00 35.14	A	C
ATOM	3611		RG 471			30.005	1.00 35.86	A	N
ATOM	3612		IRG 471			29. 723	1.00 35.39	A	C
ATOM ATOM	3613 3614	NH1 A		39. 202 37. 747		29. 830 29. 321	1.00 37.87 1.00 36.33	A A	N N
ATOM	3615		ARG 471 ARG 471	35. 17		35.064	1.00 24.89	A A	N C
ATOM	3616		IRG 471	35. 68		35. 388	1.00 24.03	A	0
ATOM	3617		YS 472			35. 935	1.00 24.59	A	Ň
ATOM	3618		YS 472			37. 373	1.00 25.55	A	Č
ATOM	3619		YS 472			37. 806	1.00 23.33	A	č .
ATOM	3620		YS 472			37. 433	1. 00 22. 34	A	ŏ
ATOM	3621		YS 472			38. 059	1.00 26.66	Ä	č
ATOM	3622		YS 472			39. 797	1.00 33.06	Ä	Š
ATOM	3623		SER 473			38. 583	1.00 22.51	Ā	Ň
ATOM	3624		ER 473			39.022	1.00 23.17	Α	C
ATOM	3625		ER 473			38. 414	1.00 21.92	A	С

				FI	G. 4	- 75			(Cont	inued)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	3626 3627 3628 3629 3630 3631 3632 3633 3634 3635 3640 3641 3642 3643 3644 3649 3650 3651 3652 3653 3656 3657 3658 3656 3657 3658	C SIGN CA CITY CON CA CITY CA	EU 477 EU 478 RO 478	39. 500 38. 557 39. 685 37. 457 37. 573 36. 330 35. 434 36. 257 35. 174 37. 280 36. 887 35. 419 37. 397 38. 294 36. 502 36. 564 37. 324 37. 925 37. 308 38. 003 37. 927 38. 661 38. 626 40. 102 37. 369 36. 160 38. 183 39. 645 37. 684 38. 908 40. 023 36. 509 36. 464 35. 561 34. 376 33. 186 31. 845	50. 976 48. 754 48. 758 48. 697 48. 627 49. 075 49. 658 48. 850 49. 389 48. 620 48. 692 46. 692 46. 692 46. 081 41. 171 40. 296 38. 851 40. 759 43. 417 43. 663 44. 505 44. 505 44. 506 42. 583 44. 600 44. 068 44. 151 43. 702	39. 071 40. 536 41. 279 42. 724 43. 459 44. 780 45. 623 45. 609 47. 022 46. 945 45. 462 46. 044 44. 691 44. 498 43. 227 42. 613 42. 818 41. 601 41. 383 42. 404 41. 943 42. 556 40. 424 40. 405 39. 428 39. 362 38. 351 37. 506 37. 116 36. 465 37. 420 36. 854	1. 00 23. 39 1. 00 23. 29 1. 00 24. 44 1. 00 23. 29 1. 00 23. 91 1. 00 24. 41 1. 00 25. 28 1. 00 24. 58 1. 00 25. 74 1. 00 24. 00 1. 00 22. 53 1. 00 25. 59 1. 00 24. 86 1. 00 26. 60 1. 00 24. 87 1. 00 24. 87 1. 00 25. 85 1. 00 27. 45 1. 00 27. 65 1. 00 27. 68 1. 00 27. 68	A A A A A A A A A A A A A A A A A A A	OCONCCONCCCONCCCONCCCCONCCCC	inued)
ATOM ATOM	3663 3664	CD1 LE	EU 479 EU 479	31. 915 30. 778	43. 702 42. 245 43. 901	36. 854 36. 430 37. 912	1.00 21.11 1.00 21.98 1.00 24.17			
ATOM ATOM ATOM ATOM ATOM ATOM ATOM	3665 3666 3667 3668 3669 3670 3671 3672 3673	C LEO	3U 479 (R 480	34. 077 33. 942 33. 978 33. 690 34. 709 36. 123 36. 702 37. 999 36. 872	44. 857 46. 073 44. 160 44. 801 44. 353 44. 657 45. 885 46. 190 43. 733	35. 199 35. 244 34. 073 32. 790 31. 749 32. 147 31. 843 32. 249 32. 870	1.00 22.18 1.00 22.27 1.00 22.51 1.00 22.76 1.00 22.59 1.00 21.95 1.00 22.81 1.00 23.84 1.00 22.05	A A A A A A	C O N C C C C C C C	
MOTA	3674	CE2 TY	TR 480	38. 165	44.027	33. 286	1.00 23.52	A	C	

										(Con	tinued)
					FΙ	G. 4	- 76			, -	
ATOM	3675	CZ	TYR	480	38. 722	45. 257	32. 971	1.00 24.29	Α	С	
ATOM	3676	0H	TYR	480	39.998	45.556	33. 379	1.00 26.37	Α	0	
ATOM	3677	C	TYR	480	32, 291	44. 422	32.326	1.00 23.22	Α	C	
ATOM	3678	0	TYR	480	31.964	43. 239	32. 243	1.00 23.21	Α	0	
ATOM	3679	N	THR	481	31.472	45. 425	32.017	1.00 23.50	Α	N	
ATOM	3680	CA	THR	481	30. 101	45. 181	31.577	1.00 22.82	Α	C	
ATOM	3681	CB	THR	481	29.097	45.513	32.702	1.00 22.81	Α	C	
ATOM	3682	0G1	THR	481	29. 190	46.905	33.024	1.00 23.28	Α	0	
ATOM	3683	CG2	THR	481	29. 398	44.699	33.951	1.00 21.29	Α	C	
ATOM	3684	C	THR	481	29.740	46.015	30.351	1.00 23.25	Α	С	
ATOM	3685	0	THR	481	30. 298	47. 091	30.136	1.00 24.47	Α	0	
ATOM	3686	N	LEU	482	28. 809	45. 512	29.547	1.00 23.21	Α	N	
ATOM	3687	CA	LEU	482	28. 368		28.350	1.00 23.54	Α	C	
ATOM	3688	CB	LEU	482	28.310	45. 268	27. 155	1.00 22.93	Α	С	
ATOM	3689	CG	LEU	482	28. 216	45.922	25.773	1.00 23.14	Α	C	
ATOM	3690		LEU	482	29. 483	46. 721	25. 507	1.00 23.20	Α	С	
ATOM	3691		LEU	482	28. 043	44. 861	24.699	1.00 22.53	Α	C	
ATOM	3692	C	LEU	482	26. 981	46. 767	28.643	1.00 23.83	Α	C	
ATOM	3693	0	LEU	482	26. 254	46. 207	29. 458	1.00 25.57	Α	0	
ATOM	3694	N	HIS	483	26. 610	47.861	27. 994	1.00 22.84	Α	N	
ATOM	3695	CA	HIS	483	25. 301	48. 459	28. 231	1.00 22.49	Α	C	
ATOM	3696	CB	HIS	483	25. 420	49. 528	29. 321	1.00 22.16	Α	C	
ATOM	3697	CG	HIS	483	26.003	49. 025	30.604	1.00 24.44	Α	C	
ATOM	3698		HIS	483	27. 289	48. 904	31.012	1.00 25.98	Α	C	
ATOM	3699		HIS	483	25. 228	48. 567	31.648	1.00 25.15	Α	N	
ATOM	3700		HIS	483	26. 011	48. 189	32.644	1.00 23.97	Α	C	
ATOM	3701		HIS	483	27. 266	48. 382	32. 283	1.00 22.74	A	N	
ATOM	3702	C	HIS	483	24. 764	49.097	26. 950	1.00 22.46	A	C	
ATOM	3703	0	HIS	483	25. 507	49. 281	25. 987	1.00 24.72	A	0	
ATOM	3704	N	SER	484	23. 475	49. 427	26. 932	1.00 20.23	A	N	
ATOM	3705	CA	SER	484	22. 890	50.078	25. 768	1.00 19.27	A	C	
ATOM	3706	CB	SER	484	21. 789	49. 216	25. 164	1.00 19.99	A	C	
ATOM	3707	0G	SER	484	20. 721	49.057	26.068	1.00 26.06	A	0	
ATOM	3708	C	SER	484	22. 335	51.427	26. 213	1.00 19.12	A	C	
ATOM	3709	0	SER	484	21.656	51. 521	27. 232	1.00 19.17	A	0	
ATOM	3710	N	SER	485	22. 628	52. 470	25. 445	1.00 19.29	A	N	
ATOM	3711	CA	SER	485	22. 198	53. 823	25. 783	1.00 20.52	A	C	
ATOM	3712 3713	CB	SER	485	23. 025	54.841	25.000	1.00 20.72	A	C	
ATOM		OG C	SER	485	24. 386	54.769	25. 379	1.00 23.68	A	0	
ATOM	3714	C	SER	485	20. 727	54.160	25. 604	1.00 20.05	A	C	
ATOM	3715 3716	0 N	SER VAL	485	20. 208	55.040	26. 287	1.00 18.92	A	0	
ATOM ATOM	3717	CA	VAL	486 486	20.055	53. 477 53. 764	24. 688	1.00 20.23	A	N	
ATOM	3718	CB	VAL	486	18.653		24. 444	1.00 19.23	A	C	
ATOM	3719		VAL	486 486	18. 058 18. 099	52.816	23. 380 23. 869	1.00 19.24	A	C	
ATOM	3720		VAL	486	16. 635	51. 383 53. 223	23. 070	1.00 19.40 1.00 20.10	A A	C	
ATOM	3721	C	VAL	486	17. 817	53. 655	25. 705	1.00 20.10	A A	C	
ATOM	3722	ŏ	VAL	486	16.869	54. 415	25. 887	1.00 19.72	A	0	
ATOM	3723	N	ASN	487	18. 190	52. 727	26. 581	1.00 20.30	A	N	
111 0111			11011	101	10.190	00.101	70. 00I	1.00 40.00	п	11	

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					(Continued)
				FIG. 4-78	
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	3773 3774 3775 3776 3777 3778 3779 3780 3781 3782 3783 3784 3785 3786 3787 3788 3789 3790 3791	CB VAL CG1 VAL CG2 VAL C VAL N LEU CA LEU CG LEU CD1 LEU CD2 LEU C LEU O LEU N GLU CA GLU CG GLU	493 493 493 493 493 494 494 494 494 495 495 495 495 495 495	29. 018	C C C C C C C C C C C C C C C C C C C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	3791 3792 3793 3794 3795 3796 3797 3798 3799 3800 3801 3802 3803 3804 3805 3806 3807 3808 3809 3810	OE1 GLU OE2 GLU C GLU N ASP CA ASP CB ASP OD1 ASP OD2 ASP O ASP N ASN CA ASN CB ASN CG ASN OD1 ASN OD ASN OD ASN O ASN	495 495 495 496 496 496 496 497 497 497 497 497	37. 539 37. 962 31. 596 1. 00 30. 56 A 34. 357 40. 210 33. 951 1. 00 25. 32 A 34. 146 41. 380 34. 285 1. 00 24. 97 A 34. 358 39. 197 34. 809 1. 00 25. 38 A 34. 093 39. 409 36. 224 1. 00 27. 01 A 32. 761 38. 757 36. 602 1. 00 27. 17 A 32. 814 37. 236 36. 567 1. 00 27. 71 A 31. 755 36. 611 36. 759 1. 00 30. 85 A 33. 898 36. 657 36. 360 1. 00 29. 23 A 35. 213 38. 889 37. 127 1. 00 27. 65 A 35. 177 39. 071 38. 345 1. 00 27. 02 A 36. 201 38. 234 36. 528 1. 00 27. 52 A 37. 329 37. 717 37. 287 1. 00 29. 40 A 38. 973 39. 622 37. 080 1. 00 29. 26 A 39. 988 39. 093 36. 630 1. 00 27. 48 A 38. 628 <	0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	3811 3812 3813 3814 3815 3816 3817 3818 3819 3820 3821	N SER CA SER CB SER OG SER C SER N ALA CA ALA CB ALA C ALA O ALA	498 498 498 498 498 499 499 499 499	36. 108 35. 721 37. 869 1. 00 31. 77 A 35. 666 34. 629 38. 716 1. 00 31. 32 A 34. 644 33. 778 37. 974 1. 00 32. 01 A 33. 520 34. 561 37. 629 1. 00 35. 01 A 36. 854 33. 772 39. 093 1. 00 30. 55 A 37. 056 33. 456 40. 266 1. 00 31. 44 A 37. 638 33. 398 38. 087 1. 00 29. 46 A 38. 814 32. 566 38. 304 1. 00 29. 07 A 39. 626 32. 477 37. 033 1. 00 27. 47 A 39. 657 33. 156 39. 421 1. 00 30. 28 A 39. 885 32. 515 40. 447 1. 00 30. 98 A	N C C O C O N C C C

		FIG	. 4 - 79		(Continued)
ATOM 3822 ATOM 3823 ATOM 3824 ATOM 3825 ATOM 3826 ATOM 3826 ATOM 3827 ATOM 3828 ATOM 3830 ATOM 3831 ATOM 3833 ATOM 3834 ATOM 3835 ATOM 3836 ATOM 3836 ATOM 3836 ATOM 3837 ATOM 3838 ATOM 3840 ATOM 3841 ATOM 3841 ATOM 3844 ATOM 3844 ATOM 3845 ATOM 3846 ATOM 3846 ATOM 3846 ATOM 3847 ATOM 3848 ATOM 3848 ATOM 3848 ATOM 3846 ATOM 3846 ATOM 3850 ATOM 3850 ATOM 3851 ATOM 3853 ATOM 3853 ATOM 3853 ATOM 3856 ATOM 3856 ATOM 3857 ATOM 3858	CA LEU CB LEU CG LEU CD1 LEU CD2 LEU CD2 LEU N ASP CA ASP CB ASP CG ASP OD1 ASP CD2 ASP CD3 ASP CD4 ASP CD5 ASP CD6 ASP CD7 ASP CD8 ASP CD8 ASP CD9 AS	500 40.098 3 500 40.919 3 500 41.218 3 500 42.106 3 500 42.269 3 500 40.251 3 500 40.251 3 501 38.984 3 501 36.815 3 501 36.349 3 501 36.349 3 501 36.349 3 501 36.349 3 501 36.349 3 501 36.349 3 501 36.349 3 501 36.349 3 501 36.349 3 501 38.432 3 502 38.470 3 502 38.470 3 502 37.853 2 502 37.783 2 502 37.783 2 502 37.783 2 502 37.783 2 503	34. 393 39. 223 45. 073 40. 208 46. 502 39. 755 47. 312 40. 703 46. 635 40. 871 48. 711 40. 155 49. 64. 772 42. 578 44. 772 42. 578 45. 44. 624 42. 905 45. 859 42. 720 45. 870 44. 831 5. 076 44. 300 4. 149 43. 557 4. 039 44. 765 3. 103 42. 740 1. 741 43. 237 0. 746 42. 100 9. 323 42. 548 8. 557 43. 050 7. 147 43. 516 7. 155 44. 696 1. 534 43. 828 1. 079 44. 963 1. 881 43. 064 1. 735 43. 528 2. 193 42. 444 1. 332 41. 200 2. 004 39. 952 1. 226 40. 438 2. 530 44. 807 1. 990 45. 790 3. 815	1.00 31.89 1.00 31.32 1.00 31.18 1.00 29.43 1.00 31.85 1.00 33.26 1.00 33.38 1.00 35.48 1.00 38.46 1.00 40.04 1.00 42.67 1.00 44.51 1.00 44.51 1.00 39.76 1.00 39.03 1.00 41.28 1.00 42.62 1.00 44.22 1.00 45.49 1.00 47.22 1.00 47.33 1.00 47.33 1.00 43.11 1.00 43.40 1.00 42.72 1.00 43.17 1.00 43.35 1.00 43.17 1.00 43.35 1.00 43.17 1.00 43.35 1.00 43.35 1.00 43.35 1.00 44.36 1.00 52.89 1.00 41.81 1.00 40.44 1.00 41.12 1.00 42.37 1.00 42.37 1.00 41.90 1.00 42.42 1.00 41.70 1.00 40.64	A
	CD2 LEU 5 C LEU 5 O LEU 5 N GLN 5 CA GLN 5 CB GLN 5	504 42. 277 38 504 41. 727 34 504 42. 056 34 505 40. 774 33 505 40. 053 32 505 38. 911 31	8. 376	1.00 40.64 1.00 43.78 1.00 43.47 1.00 44.74 1.00 45.12 1.00 47.10	A C A C A O A N A C .
ATOM 3866 ATOM 3868 ATOM 3869 ATOM 3870	CD GLN 5 OE1 GLN 5 NE2 GLN 5	505 37. 091 33 505 36. 320 33 505 37. 390 34	3. 544 48. 005 3. 143 48. 878 4. 829 47. 848		N N

		FI	G. 4-81		(Continued)
ATOM 3920 ATOM 3921 ATOM 3922 ATOM 3923 ATOM 3924 ATOM 3926 ATOM 3926 ATOM 3927 ATOM 3928 ATOM 3930 ATOM 3931 ATOM 3931 ATOM 3931 ATOM 3933 ATOM 3934 ATOM 3936 ATOM 3936 ATOM 3937 ATOM 3938 ATOM 3938 ATOM 3938 ATOM 3938 ATOM 3938 ATOM 3940 ATOM 3941 ATOM 3941 ATOM 3942 ATOM 3944 ATOM 3944 ATOM 3944 ATOM 3945 ATOM 3946 ATOM 3946 ATOM 3946 ATOM 3947 ATOM 3948	CD LYS CE LYS NZ LYS O LYS O LYS CA LYS CB LYS CG LYS CD LYS CE LYS NZ LYS C LYS O LYS C LYS O LYS C LYS O LYS C LYS O L	512 42. 252 512 42. 368 512 42. 639 512 42. 779 512 41. 095 513 41. 546 513 40. 661 513 40. 202 513 38. 754 513 40. 806 513 41. 918 514 39. 688 514 39. 688 514 39. 688 514 39. 147 514 38. 866 514 39. 435 515 39. 435 515 38. 581 515 37. 419 515 37. 278 515 36. 639	G. 4 - 8 1 50. 043	1.00 21.07 21.07 21.00 19.46 31.00 15.68 31.00 24.25 31.00 23.45 31.00 25.28 41.00 25.28 41.00 26.65 41.00 27.55 41.00 33.11 41.00 35.12 71.00 28.66 71.00 28.66 71.00 28.66 71.00 28.66 71.00 28.66 71.00 29.88 71.00 20.88 71.00 20.88 71.00 20.94 71.00 20.94 71.00 20.94 71.00 20.94 71.00 20.94 71.00 20.94 71.00 20.94 71.00 20.94 71.00 20.94 71.00 20.94 71.00 20.94 71.00 20.94 71.00 20.94 71.00 20.94 71.00 20.94 71.00 20.94 71.00 20.94	A C C A C C A C C A C C C A C C C A C C C A C C C A C C C A C C C A C C C A C C C A C C C C A C
ATOM 3941 ATOM 3942 ATOM 3943 ATOM 3944 ATOM 3945 ATOM 3946 ATOM 3947	C LEU O LEU N ASP CA ASP CB ASP OD1 ASP OD2 ASP O ASP O ASP N PHE CA PHE CB PHE CCD1 PHE CD2 PHE CD2 PHE CCE2 PHE CCE2 PHE CCZ PHE CC PHE	514 38. 812 514 37. 591 515 39. 435 515 38. 693 515 38. 581 515 37. 419 515 37. 278	55. 151 53. 788 54. 981 53. 844 56. 132 54. 437 57. 076 55. 268 56. 535 56. 693 57. 142 57. 458 56. 851 58. 668 57. 905 56. 851 58. 462 55. 287 58. 835 54. 357 59. 230 56. 345 60. 566 56. 431 61. 590 55. 729 61. 658 56. 291	3 1.00 22.73 1.00 20.65 7 1.00 23.05 8 1.00 25.43 8 1.00 27.35 8 1.00 30.82 8 1.00 32.73 1.00 32.89 7 1.00 26.80 7 1.00 27.23 1.00 27.53 1.00 27.53 1.00 28.71 1.00 28.60 1.00 28.84 1.00 29.59 1.00 29.88 1.00 29.42 1.00 26.80 1.00 28.68 1.00 27.66	A C A O A N A C A C A C A C A O
ATOM 3966 ATOM 3967 ATOM 3968	CG1 ILE CD1 ILE	517 43. 538 517 43. 676 517 40. 829	62. 861 58. 581 64. 361 58. 431 64. 132 59. 041	1.00 29.30 1.00 31.79	A C A C A C

										(Continued)
					F·I	G.	4 - 82			(Continued)
						· • ·				
ATOM	3969	0	ILE	517	40.813					0
ATOM	3970	N	IĻE	518	40.616					N
ATOM	3971	CA	ILE	518	40. 323					C
ATOM	3972	CB	ILE	518	38. 977					C
ATOM	3973	CG2		518	38.603					C
ATOM	3974	CG1		518	37. 871					C
ATOM	3975	CD1		518	36. 53					C
ATOM	3976	C	ILE	518	41.41					C
ATOM	3977	0	ILE	518	41.88					0
ATOM	3978	N	LEU	519	41.82					N
ATOM	3979		LEU	519	42.850					C
ATOM	3980	CB	LEU	519	44. 169					C
ATOM	3981		LEU	519	44. 741					C
ATOM	3982	CD1		519	45. 99					C C
ATOM	3983	CD2		519 510	45.06					Č
ATOM	3984	C	LEU	519 510	42. 35 42. 10					Õ
ATOM	3985 3986	O N	LEU ASN	519 520	42. 19					N
ATOM ATOM	3987	CA	ASN	520 520	41.73					Č
ATOM	3988	CB	ASN	520 520	42. 76					č
ATOM	3989	CG	ASN	520	44. 07					č
ATOM	3990		ASN	520	44. 54					Ŏ
ATOM	3991	ND2		520	44.69					N
ATOM	3992	C	ASN	520	40. 38					C
ATOM	3993	Ō	ASN	520	40.18					0
ATOM	3994	N	GLU	521	39.46	71.9	60.210			N
ATOM	3995	CA	GLU	521	38.10	71.8	51 59.691			C
ATOM	3996	CB	GLU	521	37.44					C
ATOM	3997	CG	GLU	521	37.96					C
ATOM	3998	CD	GLU	521	38.05					C
ATOM	3999		GLU	521	36.99					0
ATOM	4000		GLU	521	39. 19					0
ATOM	4001	C	GLU	521	38.04					C
ATOM	4002	0	GLU	521	36.96					0
ATOM	4003	N	THR	522	39.18					N C
ATOM	4004.	CA	THR	522	39. 20					C
ATOM	4005	CB	THR	522	40. 33					C 0
ATOM	4006	0G1	THR	522 522	40. 12 40. 36					C
ATOM ATOM	4007 4008	C	THR THR	522 522	39. 35					Č
ATOM	4009	0	THR	522	40.08					ŏ
ATOM	4010	N	LYS	523	38. 65			1.00 33.0		Ň
ATOM	4011	CA	LYS	523	38. 68			1.00 30.6		Ċ
ATOM	4012	CB	LYS	523	37. 35					č
ATOM	4013	CG	LYS	523	36.88					č
ATOM	4014	CD	LYS	523	35.47					Č
ATOM	4015	CE	LYS	523	34. 47					C
ATOM	4016	NZ	LYS	523	33. 11					N
ATOM	4017	C	LYS	523	39.84				84 A	C
•								001		

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								٠		(Continued)
					FI	G. 4	- 83			
ATOM	4018	0	LYS	523	39.962	66.661	53. 448	1.00 29.90	A	0
ATOM	4019	N	PHE	524	40. 711	65. 329	55.086	1.00 26.11	A	N
ATOM	4020	CA	PHE	524	41.857	64.858	54. 334	1.00 23.17	A	C
ATOM	4021	CB	PHE	524	43. 139	65. 407 66. 854	54. 953 54. 636	1.00 22.95 1.00 21.35	A A	C C
ATOM	4022	CG CD1	PHE	524 524	43. 394 43. 773	67. 242	54. 050 53. 346	1.00 21.33	A	Č
ATOM ATOM	4023 4024	CD1		524 524	43. 113	67. 830	55. 620	1.00 18.86	A	č
ATOM	4025	CE1		524	44. 026	68. 587	53. 040	1.00 19.22	Ä	č
ATOM	4026	CE2		524	43. 512	69.171	55. 329	1.00 19.37	A	C
ATOM	4027	CZ	PHE	524	43.895	69.552	54.034	1.00 19.34	Α	C
ATOM	4028	С	PHE	524	41.872	63.337	54. 328	1.00 23.15	A	·C
ATOM	4029	0	PHE	524	42.084	62. 703	55. 356	1.00 22.01	Ą	0
ATOM	4030	N	TRP	525	41.640	62. 758	53. 156	1.00 24.00	A	N
ATOM	4031	CA	TRP	525	41.593	61.309	53.000	1.00 23.65	A	C
ATOM	4032	CB	TRP	525	40. 875 39. 476	60.958 61.452	51.696 51.647	1.00 23.74 1.00 24.69	A A	C C
ATOM ATOM	4033 4034	CG CD2	TRP	525 525	38. 291	60. 687	51. 893	1.00 24.03	A	Č
ATOM	4035	CE2		525	37. 195	61.572	51.800	1.00 26.02	A	č
ATOM	4036	CE3		525	38. 049	59. 339	52. 186	1.00 25.53	A	Č
ATOM	4037	CD1		. 525	39.065	62.732	51.418	1.00 25.58	Α	С
ATOM	4038	NE1	TRP	525	37.693	62.815	51.508	1.00 25.32	Α	N
ATOM	4039	CZ2		525	35.874	61.151	51.990	1.00 25.72	Α	С
ATOM	4040	CZ3		525	36. 735	58. 919	52. 374	1.00 24.54	A	C
ATOM	4041	CH2		525	35.666	59. 824	52. 276	1.00 24.86	A	C
ATOM	4042	C	TRP	525	42.927	60.566	53. 042	1.00 23.39	A	C
ATOM ATOM	4043 4044	O N	TRP TYR	525 526	43. 994 42. 840	61. 127 59. 280	52. 803 53. 347	1.00 24.19 1.00 22.63	A A	O N
ATOM	4044	CA	TYR	526	44.002	58. 412	53. 410	1.00 22.38	A	Č
ATOM	4046	CB	TYR	526	44.715	58. 546	54. 763	1.00 22.15	Ä	Č
ATOM	4047	CG	TYR	526	43.946	57. 946	55. 929	1.00 24.08	Ä	Č
ATOM	4048	CD1	TYR	526	43.968	56. 574	56.178	1.00 23.01	Α	C .
ATOM	4049		TYR	526	43. 215	56.017	57. 204	1.00 25.01	Α	C
ATOM	4050		TYR	526	43. 150	58. 748	56. 747	1.00 24.62	A	C
ATOM	4051		TYR	526	42. 395	58. 205	57. 772	1.00 24.74	A	C
ATOM	4052	CZ	TYR	526	42.426	56.840	57. 997	1.00 25.67	A	C
ATOM	4053	OH	TYR	526	41.650	56. 303	59.003	1.00 25.43	A	0
ATOM ATOM	4054 4055	C	TYR TYR	526 526	43. 478 42. 294	56. 990 56. 724	53. 251 53. 482	1.00 22.00 1.00 21.71	A A	C 0
ATOM	4056	O N	GLN	527	44. 353	56. 084	52. 843	1.00 19.68	A	N
ATOM	4057	CA	GLN	527	43. 964	54. 697	52. 707	1.00 20.14	Ä	Ċ
ATOM	4058	CB	GLN	527	43. 842	54. 301	51. 238	1.00 19.56	A	č
ATOM	4059	CG	GLN	527	45. 123	54. 422	50. 465	1.00 23.06	A	C
ATOM	4060	CD	GLN	527	44.986	53.890	49.065	1.00 23.49	Α	C
ATOM	4061	0E1		527	44.034	54. 222	48. 359	1.00 25.79	A	0
ATOM	4062		GLN	527	45. 937	53.066	48. 648	1.00 22.35	A	N
ATOM	4063	Ç	GLN	527	45.038	53. 871	53. 389	1.00 20.67	A	C
ATOM	4064	0 N	GLN	527	46. 172	54. 334	53. 563	1.00 19.72	A	0 N
ATOM	4065 4066	N CA	MET	528 528	44.674	52. 659 51. 771	53. 792 54. 460	1.00 21.11 1.00 22.32	A A	N C
ATOM	4000	UA	MET	Ų40	45. 610	01. ((1	04. 400	1.00 44.04	n	U

(Continued)											
				FIG. 4-84							
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	4068 C 4069 S 4070 C 4071 C 4072 C 4073 N 4074 C 4075 C 4076 C 4077 C 4078 C 4077 C 4078 C 4079 C 4080 C 4081 N 4082 C 4083 C 4084 C 4085 C 4086 C 4087 C 4088 C 4088 C 4089 C 4090 C 4091 C 4092 C 4093 C 4094 C 4095 C 4096 C 4097 C 4098 C 4099 C 4098 C	MET ILE ILE CA ILE CG2 ILE CG1 ILE CG1 ILE CD1 ILE CD1 ILE CD2 LEU CCA LEU CCD2 LEU CCD2 LEU CCD2 LEU CCD2 LEU CCD PRO	528 528 528 528 529 529 529 529 529 529 530 530 530 531 531 531 531 532 532 532 532	FIG. 4 - 84 45. 372 51. 753 55. 967 1. 00 23. 57 45. 830 52. 971 56. 727 1. 00 23. 53 45. 605 52. 683 58. 492 1. 00 23. 56 46. 400 54. 107 59. 158 1. 00 21. 91 45. 482 50. 347 53. 974 1. 00 23. 25 44. 383 49. 790 53. 935 1. 00 24. 82 46. 605 49. 751 53. 600 1. 00 22. 51 46. 587 48. 363 53. 183 1. 00 21. 97 47. 644 48. 078 52. 116 1. 00 19. 54 47. 557 46. 635 51. 681 1. 00 18. 75 47. 454 49. 029 50. 927 1. 00 21. 01 46. 045 49. 038 50. 335 1. 00 19. 28 46. 937 47. 620 54. 465 1. 00 24. 02 48. 114 47. 505 54. 820 1. 00 25. 51 45. 911 47. 153 55. 175 1. 00 24. 47 46. 114 46. 443 56. 438 1. 00 24. 76 44. 915 46. 640 57. 370 1. 00 24. 08 44. 451 48. 052 57. 726 1. 00 24. 08 44. 451 48. 052 57. 726 1. 00 24. 92 43. 365 47. 928 58. 763 1. 00 24. 92 44. 366 44. 319 55. 411 1. 00 24. 39 45. 686 44. 319 55. 411 1. 00 24. 39 46. 337 44. 953 56. 241 1. 00 24. 58 47. 272 44. 374 57. 003 1. 00 24. 58 48. 174 45. 045 57. 950 1. 00 24. 42 47. 578 42. 943 56. 913 1. 00 26. 79 48. 763 42. 784 57. 862 1. 00 26. 36 48. 580 43. 913 58. 838 1. 00 26. 79 48. 763 42. 784 57. 862 1. 00 28. 05 46. 388 42. 078 57. 312 1. 00 28. 05 45. 443 42. 562 57. 931 1. 00 31. 01 46. 417 40. 782 56. 964 1. 00 28. 68 45. 783 38. 534 56. 745 1. 00 28. 68	CCSCCONCCCCCONCCCCONCCCCONCCCC						
ATOM ATOM ATOM	4100 4101	CG PRO C PRO O PRO	532 532 532	46.726 38.912 55.659 1.00 28.50 A 45.113 39.799 58.814 1.00 29.80 A 46.051 40.006 59.579 1.00 31.52 A	C C						
ATOM ATOM ATOM ATOM	4103 4104 4105 4106	N HIS CA HIS CB HIS CG HIS	533 533 533 533	43.894 39.501 59.242 1.00 31.29 A 43.605 39.382 60.670 1.00 31.80 A 44.278 38.127 61.225 1.00 29.82 A 44.170 36.936 60.324 1.00 29.23 A	C C C						
ATOM ATOM ATOM ATOM ATOM	4108 4109 4110 4111	CD2 HIS ND1 HIS CE1 HIS NE2 HIS C HIS	533 533 533 533	45.114 36.247 59.641 1.00 28.40 A 42.966 36.335 60.024 1.00 28.40 A 43.174 35.326 59.197 1.00 28.67 A 44.469 35.251 58.949 1.00 28.85 A 44.101 40.601 61.445 1.00 33.77 A 44.469 40.489 62.617 1.00 33.99 A	A N A C A N A C						
ATOM ATOM ATOM ATOM	4113 4114	O HIS N PHE CA PHE CB PHE	533 534 534 534	44. 469 40. 489 62. 617 1. 00 33. 99 44. 121 41. 758 60. 787 1. 00 35. 52 44. 578 42. 987 61. 427 1. 00 37. 29 44. 249 44. 203 60. 555 1. 00 36. 11	A N A C						

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					7.1		0.5			(Continued)
					FIC	G. 4	- 85			
ATOM	4116	CC	מוומ	E94	44 E10	45. 523	61. 235	1.00 35.46	٨	C
ATOM	4116 4117	CC	PHE PHE	534 534		45. 956	61.475	1.00 35.40	A A	C C
ATOM	4117		PHE	534 534		46. 320	61.654	1.00 33.35	A	Č
ATOM ATOM	4119		PHE	534 534		47. 167	62. 124	1.00 36.55	A	Č
ATOM	4119		PHE	534		47. 530	62. 304	1.00 35.26	A	č
ATOM	4121	CZ	PHE	534		47. 957	62. 541	1.00 35.35	A	č
ATOM	4122	C	PHE	534		43. 158	62. 790	1.00 38.07	A	č
ATOM	4123	Ö	PHE	534		43.046	62. 911	1.00 38.83	A	ŏ
ATOM	4124	N	ASP	535		43. 435	63. 810	1.00 39.27	A	N
ATOM	4125	CA	ASP	535		43. 621	65. 160	1.00 40.72	A	Ċ
ATOM	4126	CB	ASP	535		42. 541	66.089	1.00 43.14	A	Č
ATOM	4127	CG	ASP	535		42. 571	67.460	1.00 46.19	A	C
ATOM	4128		ASP	535		43.668	67.912	1.00 46.58	Α	0
ATOM	4129		ASP	535		41.499	68.092	1.00 48.00	Α	0
ATOM	4130	C	ASP	535		44.985	65.699	1.00 40.91	Α	C
ATOM	4131	0	ASP	535		45.270	65.837	1.00 40.57	Α	0
ATOM ·	4132	N	LYS	536		45.822	66.022	1.00 41.40	Α	N
ATOM	4133	CA	LYS	536	43. 936	47.148	66.539	1.00 42.56	· A	C
ATOM	4134	CB	LYS	536		48.018	66.572	1.00 44.69	Α	С
ATOM	4135	CG	LYS	536		48.406	65.200	1.00 47.06	Α	C
ATOM	4136	CD	LYS	536		49. 566	65. 289	1.00 49.52	Α	C
ATOM	4137	CE	LYS	536		50.020	63.897	1.00 50.85	A	С
ATOM	4138	NZ	LYS	536		51.303	63. 921	1.00 51.05	Ą	N
ATOM	4139	C	LYS	536		47.105	67. 928	1.00 42.57	A	C
ATOM	4140	0	LYS	536		48. 147	68.486	1.00 42.20	A	0
ATOM	4141	N	SER	537		45.907	68. 486	1.00 42.80	A	N
ATOM	4142	CA	SER	537		45. 762	69. 820	1.00 43.70	A	C
ATOM	4143	CB	SER	537		44. 499	70. 513	1.00 44.09	A	C
ATOM	4144	OG C	SER	537		43.319	69. 888	1.00 43.50	A	0
ATOM	4145	C	SER	537 537		45.696	69. 737 70. 682	1.00 43.27 1.00 44.98	A	C 0
ATOM ATOM	4146 4147	O N	SER Lys	538		46. 061 45. 230	68. 598	1.00 44.98	A	N N
ATOM	4148	CA	LYS	538		45. 110	68. 380	1.00 41.33	A A	C
ATOM	4149	CB	LYS	538		43. 917	67. 470	1.00 40.13	A	Č
ATOM	4150	CG	LYS	538		42. 590	68. 013	1.00 41.23	A	č
ATOM	4151	CD	LYS	538		41.446	67. 073	1.00 41.97	A	č
ATOM	4152	CE	LYS	538		40. 140	67. 638	1.00 42.57	A	č
ATOM	4153	NZ	LYS	538		40. 231	67.960	1.00 44.10	A	Ň
ATOM	4154	C	LYS	538		46. 372	67. 741	1.00 38.59	Ä	Ċ
ATOM	4155	ŏ	LYS	538		47. 229	67. 283	1.00 38.17	Ä	Ö
ATOM	4156	Ň	·LYS	539		46. 485	67. 725	1.00 36.92	A	N
ATOM	4157	CA	LYS	539		47.629	67.116	1.00 36.43	Ā	C
ATOM	4158	CB	LYS	539		48. 225	68.079	1.00 37.32	Ā	Č
ATOM	4159	CG	LYS	539		48.838	69.341	1.00 37.42	Α	C
ATOM	4160	CD	LYS	539		50.117	69.028	1.00 40.01	Α	C
ATOM	4161	CE	LYS	539		50.674	70. 258	1.00 41.64	Α	C
ATOM	4162	NZ	LYS	539		51.014	71.389	1.00 43.98	Α	N
ATOM	4163	C	LYS	539		47.110	65. 849	1.00 35.38	A	C
ATOM	4164	0	LYS	539	52. 699	46.137	65. 893	1.00 35.49	A	0

(Continued)

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	•			FIC	G. 4-	8 6			Continued
4 TO14	ALCE N	TYR	540	51.658	47. 747	64. 719	1.00 33.00	Α	N
ATOM	4165 N 4166 CA	TYR	540 540	52. 229	47. 316	63. 452	1.00 30.12	Α	C
ATOM ATOM	4160 CA 4167 CB	TYR	540	51.131	47. 135	62.397	1.00 28.99	Α	С
ATOM	4167 CB	TYR	540	50. 204	45.968	62.630	1.00 29.13	Α	С
ATOM		TYR	540	49.109	46.078	63.488	1.00 28.32	Α	C
ATOM		TYR	540	48. 254	45.000	63.699	1.00 27.13	A	C
ATOM		TYR	540	50. 421	44.748	61.990	1.00 27.62	A	C
ATOM	4172 CE2		540	49.576	43.669	62.196	1.00 26.32	A	C
ATOM	4173 CZ	TYR	540	48.495	43.800	63.051	1.00 27.64	A	C
ATOM	4174 OH	TYR	540	47.661	42.724	63.260	1.00 29.67	A	0
ATOM	4175 C	TYR	540	53. 242	48. 287	62.890	1.00 29.33	A	C
ATOM	4176 0	TYR	540	53.130	49.492	63. 091	1.00 31.23	A	0
ATOM	4177 N	PR0	541	54.270	47.772	62. 199	1.00 27.71	A	N
ATOM	4178 CD	PR0	541	54.717	46. 383	62.020	1.00 25.95	A	C
ATOM	4179 CA	PRO	541	55. 238	48. 708	61.634	1.00 27.56	A	C
ATOM	4180 CB	PR0	541	56. 361	47. 794	61.148	1.00 26.81	A	C
ATOM	4181 CG	PRO	541	55.662	46. 512	60.867	1.00 25.92	A	C C
ATOM	4182 C	PRO	541	54. 463	49. 358	60.500	1.00 27.83	A	0
ATOM	4183 0	PRO	541	53. 579	48. 727	59. 912	1.00 28.03	A	N
ATOM	4184 N	LEU	542	54. 763	50.613	60. 200	1.00 27.70	A A	C
ATOM	4185 CA	LEU	542	54.032	51.307	59. 154	1.00 26.55 1.00 26.11	A	Č
ATOM	4186 CB	LEU	542	53. 220	52.440	59. 791	1.00 20.11	A	Č
ATOM	4187 CG	LEU	542	52. 252	53. 292	58. 959 59. 898	1.00 29.38	A	Č
ATOM		LEU	542	51.422 53.017	54. 170 54. 165	57. 979	1.00 29.52	A	Č
ATOM		LEU	542	54. 924	51.855	58. 042	1.00 26.16	A	Č
ATOM	4190 C	LEU	542	55. 943	52. 492	58. 303	1.00 28.00	Ä	ŏ
ATOM	4191 0	LEU LEU	542 543	54. 536	51. 589	56.801	1.00 23.70	Ä	Ň
ATOM	4192 N 4193 CA	LEU	543	55. 263	52.097	55.651	1.00 24.11	A	Ċ
ATOM	4193 CA 4194 CB	LEU	543	55. 595	50. 978	54.660	1.00 24.05	Ā	Č
ATOM ATOM	4194 CB 4195 CG	LEU	543	56.080	51.474	53. 289	1.00 22.45	A	C C
ATOM		LEU	543	57. 209	52. 487	53. 475	1.00 24.00	Α	C
ATOM		LEU LEU	543	56. 537	50. 303	52.441	1.00 20.16	Α	C
ATOM	4198 C	LEU	543	54. 378	53. 131	54.966	1.00 24.37	Α	C
ATOM	4199 0	LEU	543	53. 283	52.819	54.511	1.00 25.72	Α	0
ATOM	4200 N	LEU	544	54.857	54.362	54.896	1.00 24.80	Α	N
ATOM	4201 CA	LEU	544	54.098	55.436	54.278	1.00 23.74	A	C
ATOM	4202 CB		544	54.424	56.757	54.979	1.00 23.92	Α	С
ATOM	4203 CG		544	53.640	58.003	54. 581	1.00 22.62	A	C
ATOM		1 LEU	544	52.157	57.743	54.729	1.00 24.91	A	C
ATOM		2 LEU	544	54.069	59.166	55.460	1.00 24.25	A	C
ATOM	4206 C	LEU	544	54. 403		52. 785	1.00 23.24	A	C
ATOM	4207 0	LEU	544	55. 451	56.053	52.400	1.00 23.44	A	0
ATOM	4208 N	ASP	· 545	53. 477		51.962	1.00 21.43	A	N
ATOM	4209 CA		545	53. 595		50.508		A	C
ATOM	4210 CB		545	52. 570		49. 902		A	C
ATOM	4211 CG		545	52.826		48. 444		A	C
ATOM		1 ASP	545	53. 175				A	0
ATOM	4213 OD	2 ASP	545	52.660	52.675			A	0
							301		

	(Continued)						
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	4214 4215 4216 4217 4218 4219 4220 4221 4222 4223 4224 4225 4223 4231 4232 4233 4234 4235 4236 4237 4242 4243 4242 4243 4242 4243 4242 4243 4242 4243 4242 4243 4242 4243 4242 4243 4242 4243 4244 4245 4246 4247 4248 4249 4250 4251 4252 4253 4264 427 427 4288 4298 4298 4298 4298 4298 4298 4298	O N CAE CC CC CC CC CC CC CC O N CC CC O N CC C	VAL VAL VAL TYR TYR TYR TYR TYR TYR TYR TYR TYR ALA ALA ALA ALA ALA ALA ALA ALA ALA AL	54566654777777777775488888999000000000000000000000000000000	52. 653 60. 155 44. 952 1. 00 13. 49 52. 969 60. 718 43. 589 1. 00 13. 89 52. 160 61. 688 43. 006 1. 00 14. 20 52. 513 62. 274 41. 801 1. 00 13. 67 54. 136 60. 347 42. 921 1. 00 9. 92 54. 492 60. 926 41. 726 1. 00 10. 35 53. 680 61. 890 41. 167 1. 00 12. 20 54. 036 62. 474 39. 973 1. 00 14. 66 53. 522 62. 076 46. 266 1. 00 14. 99 54. 490 62. 834 46. 325 1. 00 14. 47 52. 265 62. 456 46. 479 1. 00 14. 77 51. 879 63. 806 46. 878 1. 00 12. 10 52. 493 64. 109 48. 247 1. 00 9. 78 52. 163 64. 950 45. 923 1. 00 11. 87 52. 250 66. 094 46. 346 1. 00 12. 24 52. 308 64. 660 44. 639 1. 00 13. 20 51. 306 65. 778 43. 573 1. 00 13. 15 50. 266 66. 182 <td< td=""><td>1 1 1 1</td><td>(Continued) C O N C C C C C C C C C C C C C C C C</td></td<>	1 1 1 1	(Continued) C O N C C C C C C C C C C C C C C C C
ATOM ATOM ATOM	4260 4261 4262	OG C O	SER SER SER	552 552 552 552	49. 023 63. 805 44. 987 1. 00 20. 36 A 46. 602 63. 202 43. 760 1. 00 17. 72 A 45. 723 63. 929 44. 243 1. 00 17. 55 A		C O C O
					SUBSTITUTE SHEET (RULE 26)		

(Continued)

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					FΙ	G. 4	- 88	•		(00100111111111111111111111111111111111	
ATOM	4263		GLN	553	46.632	61.885	43. 926	1.00 17.07	A	N C	
ATOM	4264	-	GLN	553	45.628	61.179	44. 699	1.00 16.87	A	C	
ATOM	4265		GLN	553	44. 301	61.090	43. 937	1.00 16.43 1.00 19.53	A A	C	
ATOM	4266		GLN	553	43. 249	60. 292	44. 695	1.00 19.55	A A	C	
ATOM	4267		GLN	553	41.844	60.468		1.00 10.67	A	0	
ATOM	4268	OE1		553	41.520	60.019	43.066	1.00 20.07	A	N	
ATOM	4269	NE2		553	40.999	61.126	44. 944 44. 996	1.00 18.07	A	C	
ATOM	4270		GLN	553	46.123 46.088	59. 781 58. 915	44. 129	1.00 18.05	A	Ö	
ATOM	4271		GLN	553 554	46.589	59. 562	46. 221	1.00 10.23	A	N	
ATOM	4272		LYS	554 554	47. 075	58. 248	46. 620	1.00 10.69	Ä	Č	
ATOM	4273		LYS LYS	554 554	48.319	58. 387	47. 490	1.00 22.65	Ä	č	
ATOM ATOM	4274 4275		LYS	554 554	49.538	58. 887	46. 733	1.00 24.15	Ä	č	
ATOM .			LYS	554	50.064		45. 765	1.00 25.21	Ä	Č	
ATOM	4277		LYS	554	50.777		46. 503	1.00 24.75	Ä	č	
ATOM	4278		LYS	554	51.472	55. 796	45. 560	1.00 23.89	A	Ň	
ATOM	4279		LYS	554	45. 996	57.472	47. 374	1.00 21.48	A	С	
ATOM	4280		LYS	554	46.108	56. 258	47.549	1.00 22.39	Α	0	
ATOM	4281	Ň	ALA	555	44.952	58.176	47.807	1.00 20.77	A	N	
ATOM	4282	CA	ALA	555	43.849	57. 555	48.538	1.00 20.46	Α	C	
ATOM	4283	CB	ALA	555	43. 525	58.376	49.768	1.00 18.05	Α	C	
ATOM	4284	C	ALA	555	42.611	57.436	47.643	1.00 21.32	Α	С	
ATOM	4285	0	ALA	555	41.996		47. 285	1.00 21.75	Α	0	
ATOM	4286	N	ASP	556	42. 249		47. 283	1.00 21.00	Α	N	
ATOM	4287	CA	ASP	556	41.096		46.419		A	C	
ATOM	4288	CB	ASP	556	41.500		44.960	1.00 20.02	A	C	
ATOM	4289	CG	ASP	556	42.649	55. 255	44. 574	1.00 19.76	A	C	
ATOM	4290		ASP	556	42. 723		45. 115	1.00 19.65	A	0	
ATOM	4291	0D2		556	43.470		43. 723	1.00 21.90	A	0	
ATOM	4292	C	ASP	556	40. 478	54. 603	46.614	1.00 20.18	A	C	
ATOM	4293	0	ASP	556	40.856		47. 523	1.00 19.93	A	0	
ATOM	4294	N	THR	557	39. 542		45. 736	1.00 20.55	A	N	
ATOM	4295	CA	THR	557	38. 835		45. 820	1.00 22.31	A	C	
ATOM	4296	CB	THR	557	37. 331	53. 154	45. 578	1.00 21.37 1.00 21.50	A A	C 0	
ATOM	4297		THR		37. 130 36. 754		44. 224 46. 523	1.00 21.30	A	C	
ATOM	4298	C	THR THR	557 557	39. 294		44. 826	1.00 21.28	A	Č	
ATOM	4299 4300			557	20 ENE	50 QQ1		1.00 25.32			
ATOM ATOM	4300	N	VAL	558	40. 441	52. 105	44. 194	1.00 22.84	A	N	
ATOM	4302	CA	VAL	558	40. 931	51. 143	43. 219	1.00 22.53	A	Č	
ATOM	4303	CB	VAL	558	41.970	51.802	42. 294	1.00 22.67	Ä	Č	
ATOM	4304		VAL	558	42. 540		41. 323	1.00 19.20	A	č	
ATOM	4305		VAL	558	41.323	52.964	41.547	1.00 21.12	A	Č	
ATOM	4306	Č	VAL	558	41.544	49.906	43.871	1.00 23.92	Α	С	
ATOM	4307	Ŏ	VAL	558	42. 246	50.005	44.871	1.00 23.71	A	. 0	
ATOM	4308	Ň	PHE	559	41.261	48. 734	43. 312	1.00 25.05	Α	N	
ATOM	4309	CA	PHE	559	41.815	47.492	43.841	1.00 25.45	Α	С	
ATOM	4310	CB	PHE	559	40.855	46.326	43. 584	1.00 24.60	Α	С	
ATOM	4311	CG	PHE	559	41.476		43. 808	1.00 24.75	Α	С	

ATOM

4360 N ALA

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(Continued) FIG. 4-89 **ATOM** 4312 CD1 PHE 559 42.192 44.352 42.799 1.00 25.70 C 41. 382 42. 810 41. 995 4313 CD2 PHE 559 1.00 25.27 **ATOM** 44.352 45.044 \mathbf{C} Α 43.021 **ATOM** 4314 CE1 PHE 559 43.118 1.00 28.04 A 43.125 45.276 C **ATOM** 4315 CE2 PHE 559 1.00 24.71 Α 42. 709 43. 158 44.266 C CZ42.507 1.00 26.38 **ATOM** 4316 PHE 559 A 47. 210 Ċ **ATOM** 4317 C 559 43.170 1.00 26.14 PHE A **ATOM** 4318 0 PHE 559 43.250 47.246 41.943 1.00 27.21 0 Α 44.188 46.912 **ATOM** 4319 N 560 43.962 1.00 24.72 ARG Α N 45. 508 43. 397 43. 510 4320 46.644 **ATOM** CA 1.00 23.52 $^{\rm C}$ ARG 560 A 47. 892 CB **ATOM** 4321 ARG 560 46.398 1.00 20.68 A $^{\rm C}_{\rm C}$ ATOM 4322 CG ARG 560 45.869 49.140 42.802 1.00 19.21 A **ATOM** 4323 CD 46.885 50.285 42.869 ARG 560 1.00 17.64 A 46. 269 45. 637 51. 536 52. 391 43. 310 **ATOM** 4324 NE 1.00 20.38 ARG N 560 A **ATOM** 4325 CZ42.515 C ARG 560 1.00 20.51 A **ATOM** 4326 NH1 ARG 45.543 52.149 41.218 1.00 26.51 560 A N 43. 022 43. 980 45.061 **ATOM** 4327 NH2 ARG 53.468 560 1.00 20.25 A N 46. 274 ATOM 4328 C 45.451 ARG 560 1.00 24.37 A C ATOM 4329 46.112 0 ARG 560 45.081 45.145 1.00 24.84 Α 0 ATOM 4330 LEU 47.111 44.856 43.136 N 561 1.00 23.62 A N 43.511 42.635 42.773 47.968 ATOM 4331 LEU 43.740 1.00 20.95 CA 561 A C 42. 523 47.680 **ATOM** 4332 LEU CB 561 1.00 18.87 A C ATOM 4333 CG LEU 561 46.283 41.916 1.00 20.60 A C CD1 LEU 40.749 **ATOM** 4334 561 46.139 41.803 C 1.00 19.75 A 44. 203 43. 246 **ATOM** 4335 CD2 LEU 46.045 41.460 Č 561 1.00 17.53 A 49. 380 **ATOM** 4336 44.255 C LEU 561 1.00 20.00 C A **ATOM** 4337 0 LEU 561 49.894 44.152 42.133 1.00 20.19 0 A ATOM 4338 ASN 49.999 44.822 N 562 44.274 1.00 18.97 Α N ASN ASN **ATOM** 51.335 45. 392 44. 142 4339 562 CA 1.00 18.20 C A ATOM ATOM 4340 CB 562 51.197 46.907 44.028 1.00 16.72 C A 4341 CG ASN 562 50.364 47.491 45.148 1.00 17.45 C A 49. 881 50. 195 **ATOM** 4342 OD1 ASN 562 48.610 45.054 1.00 19.63 0 A ND2 ASN ATOM 4343 562 46.729 46.223 1.00 18.39 N A ATOM 4344 52.291 C ASN 562 45.035 45.289 1.00 18.48 C A ATOM 4345 ASN 52.055 0 562 44.098 46.056 1.00 19.79 A 0 53. 375 54. 366 **ATOM** 4346 45.793 N TRP 563 45.400 1.00 17.98 A N TRP **ATOM** 4347 CA 563 45.548 46.434 1.00 17.62 Α C ATOM 55.538 4348 CB TRP 563 46.537 46.290 1.00 16.04 Ċ A 56. 741 57. 474 46. 249 47. 200 ATOM 4349 CG TRP 563 47.178 1.00 15.76 C A **ATOM** 4350 CD2 TRP 563 47.968 1.00 13.80 C A ATOM 4351 CE2 TRP 563 58.526 46.500 48.602 1.00 11.13 C A 57. 341 57. 367 ATOM 4352 CE3 TRP 563 48.575 48.198 1.00 13.46 A ATOM 4353 CD1 TRP 563 45.041 47.361 1.00 12.65 C A **ATOM** 4354 NE1 TRP 563 58.440 45.189 48.217 1.00 11.34 N A ATOM 4355 CZ2 TRP 563 59.439 47.128 49.453 C 1.00 14.40 A ATOM 4356 58. 252 CZ3 TRP 49.204 563 49.046 1.00 16.29 C A ATOM 4357 CH2 TRP 59.291 48.476 563 49.664 1.00 14.18 C ATOM 4358 C TRP 53.728 Č 563 45.672 47.809 1.00 17.48 A ATOM 4359 0 TRP 48.720 1.00 18.93 563 54.048 44.910 0 A

> 46.620 SUBSTITUTE SHEET (RULE 26)

47.953

1.00 16.80

N

52.813

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					FIG. 4-91	(Continued)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	4410 4411 4412 4413 4414 4415 4416 4417 4418 4420 4421 4422 4423 4424 4425 4429 4430 4431 4432 4433 4434 4435 4436 4447 4448 4449 4449	CA CB CG CD 1 OE 2 C O N CA CB CG CD 1 C O N CA CB CG CC CD 1 C C CC	VAL VAL VAL	571 571 571 571 571 571 572 572 572 572 572 573 573 573 573 573 574 574 574 574 575 575 575 575 575 575	54. 686 40. 329 55. 253 1. 00 26. 71 A 55. 480 41. 020 56. 259 1. 00 25. 23 A 56. 402 42. 040 55. 583 1. 00 24. 64 A 57. 287 41. 472 54. 473 1. 00 25. 43 A 58. 238 40. 392 54. 966 1. 00 27. 45 A 58. 582 40. 421 56. 164 1. 00 28. 11 A 58. 656 39. 527 54. 158 1. 00 27. 18 A 54. 643 41. 715 57. 329 1. 00 24. 50 A 55. 188 42. 368 58. 213 1. 00 24. 29 A 53. 324 41. 576 57. 247 1. 00 24. 39 A 52. 425 42. 191 58. 223 1. 00 24. 96 A 52. 139 40. 033 59. 569 1. 00 25. 44 A 52. 12 39. 734 58. 694 1. 00 29. 03 A 51. 128 39. 734 58. 694 1. 00 29. 67 A 52. 944 44. 387 57. 321 1. 00 25. 32 A 41. 718 <t< td=""><td></td></t<>	
ATOM ATOM	4448 4449	C 0	VAL VAL	575 575	50. 054 51. 585 53. 837 1. 00 25. 21 A 48. 929 51. 312 53. 405 1. 00 25. 63 A	C 0
ATOM ATOM ATOM ATOM ATOM ATOM	4450 4451 4452 4453 4454 4455	N CA CB C O N	ALA ALA ALA ALA SER	576 576 576 576 576 577	50. 403 52. 804 54. 216 1. 00 23. 75 A 49. 456 53. 893 54. 152 1. 00 23. 56 A 49. 255 54. 477 55. 540 1. 00 23. 43 A 49. 879 54. 988 53. 180 1. 00 24. 06 A 51. 056 55. 139 52. 860 1. 00 22. 16 A 48. 888 55. 740 52. 710 1. 00 24. 49 A	N C C C O N
ATOM ATOM ATOM	4456 4457 4458	CB	SER SER SER	577 577 577	49. 095 56. 852 51. 796 1. 00 23. 11 A 48. 793 56. 428 50. 362 1. 00 23. 06 A 49. 750 55. 475 49. 921 1. 00 22. 88 A	C C O

					- FI	G. 4	- 92			(Continue	d)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	4459 4460 4461 4462 4463 4464 4465 4466 4467 4468 4470 4471 4472 4473 4474 4475 4476 4477 4478 4479 4480 4481 4482 4483 4484 4488	CA CB CG CD1 CD2 CE1 CE2 CZ C C O N CA CB CG OD1 CA C C O N CA C C C C C C C C C C C C C C C C C	PHE PHE PHE PHE ASP ASP ASP ASP ASP ASP ASP ASP ASP ARG ARG ARG	577 578 578 578 578 578 578 578 578 578	48. 149 47. 075 48. 546 47. 748 48. 313 47. 585 46. 429 48. 080 45. 783 47. 441 46. 288 47. 723 48. 766 46. 533 46. 389 45. 191 45. 334 46. 424 44. 342 46. 211 45. 103 47. 238 47. 065 46. 544 47. 495 47. 377 47. 956 47. 072	57. 947 57. 662 59. 196 60. 337 60. 829 62. 005 61. 820 63. 291 64. 381 64. 186 61. 502 61. 909 62. 041 63. 173 62. 985 61. 777 61. 583 61. 024 64. 474 64. 823 65. 189 67. 610 67. 462 68. 786 69. 970 71. 172 71. 645	52. 248 52. 768 52. 479 53. 804 54. 383 55. 144 54. 209 55. 730 54. 790 55. 556 51. 480 50. 973 51. 212 50. 302 49. 371 48. 455 47. 873 48. 299 51. 092 51. 493 51. 313 52. 044 51. 098 49. 993 51. 528 50. 701 51. 444 52. 585	1. 00 22. 90 1. 00 24. 22 1. 00 23. 49 1. 00 21. 77 1. 00 21. 41 1. 00 22. 79 1. 00 20. 60 1. 00 19. 79 1. 00 20. 94 1. 00 20. 70 1. 00 21. 14 1. 00 21. 08 1. 00 19. 89 1. 00 18. 01 1. 00 17. 01 1. 00 21. 86 1. 00 22. 87 1. 00 23. 17 1. 00 18. 10 1. 00 20. 42 1. 00 17. 22 1. 00 15. 14 1. 00 16. 53 1. 00 15. 52 1. 00 16. 17 1. 00 16. 05 1. 00 14. 87	A A A A A A A A A A A A A A A A A A A	CONCCCCCCCCONCCCONCCCONCCC	d)
ATOM ATOM ATOM	4488 4489 4490	CD NE CZ	ARG ARG ARG	581 581 581	47. 756 48. 617 49. 321	72. 653 71. 990 72. 624	53. 467 54. 441 55. 375	1.00 14.87 1.00 18.25 1.00 19.44	A A A	C N C	
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	4491 4492 4493 4494 4495 4496 4497 4498 4499		ARG ARG ARG GLY GLY GLY SER	581 581 581 581 582 582 582 582 583	49. 268 50. 075 48. 107 49. 193 47. 495 48. 094 47. 511 47. 673 46. 842	73. 952 71. 933 69. 742 69. 158 70. 192 70. 022 68. 842 68. 757 67. 923	55. 463 56. 224 49. 386 49. 357 48. 295 46. 987 46. 231 45. 017 46. 925	1.00 20.41 1.00 15.76 1.00 17.75 1.00 17.49 1.00 18.96 1.00 17.63 1.00 18.54 1.00 18.09 1.00 18.00	A A A A A A A	N C O N C C C O	
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	4500 4501 4502 4503 4504 4505 4506 4507	CA CB OG C O N CA C	SER SER SER SER GLY GLY GLY	583 583 583 583 583 584 584 584	46. 258 45. 842 45. 058 45. 068 44. 601 44. 570 43. 481 42. 052	66. 765 65. 700 66. 253 67. 218 68. 344 66. 355 66. 779 66. 293	46. 247 47. 269 48. 303 45. 392 45. 536 44. 510 43. 637 43. 827	1.00 18.46 1.00 18.34 1.00 19.12 1.00 18.03 1.00 17.42 1.00 17.84 1.00 19.22 1.00 19.49	A A A A A A	C C O C O N C C	

									(Continued)
				FI	G. 4 -	94			(Oomminaca)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	4558 4559 4560 4561 4562 4563 4564 4565 4566 4567 4568 4569 4570 4571 4572 4573 4574 4575 4576 4577	C ILI O ILI N ME: CA ME: CB ME: CB ME: CC ME	E 590 F 591 F 591 F 591 F 591 F 591 F 591 F 591 F 592 F 592 F 592 F 592 F 592 F 592 F 592 F 592 F 592 F 593 F 594 F 595 F 595	44. 537 45. 711 44. 157 45. 127 44. 406 45. 309 44. 403 44. 237 46. 112 47. 289 45. 636 46. 502 45. 713 45. 296 45. 604 44. 471 44. 289 44. 965 47. 197 47. 842 47. 732 47. 360	72. 093 71. 960 72. 071 71. 846 71. 567 71. 000 70. 746 72. 436 72. 997 72. 771 74. 228 75. 386 76. 560 76. 361 75. 390 77. 243 76. 825 75. 703 75. 817 76. 865 75. 012 75. 349 74. 349	47. 562 47. 901 46. 291 45. 232 43. 917 42. 838 41. 309 40. 732 45. 051 44. 791 45. 200 45. 035 44. 455 43. 032 42. 139 42. 368 41. 128 40. 962 46. 319 46. 362 47. 367 48. 628 49. 710	1. 00 22. 32 1. 00 23. 51 1. 00 21. 59 1. 00 21. 80 1. 00 21. 85 1. 00 22. 76 1. 00 22. 84 1. 00 21. 43 1. 00 21. 21 1. 00 21. 21 1. 00 21. 23 1. 00 22. 32 1. 00 24. 65 1. 00 25. 75 1. 00 25. 75 1. 00 25. 78 1. 00 21. 38 1. 00 21. 38 1. 00 20. 84 1. 00 20. 84 1. 00 20. 43 1. 00 18. 24	A A A A A A A A A A A A A A A A A A A	(Continued) C O N C C C C C C C C C C C C C C C C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	4576 4577 4578 4579 4580 4581 4582 4583 4584 4585 4586 4587 4588 4589 4590 4591 4592 4593 4594 4595	O HI N AL CA AL	S 592 A 593 A 593 A 593 A 593 B 594 B 594 B 594 B 594 B 594 B 594 B 594 B 594 B 594 B 595 SN 595 SN 595 SN 595 SN 595	47. 842 47. 076 47. 732	76. 865 75. 012 75. 349	46. 362 47. 367 48. 628	1.00 20.84 1.00 21.76 1.00 20.43	A A A	O N C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	4596 4597 4598 4599 4600 4601 4602 4603 4604 4605	O AS N AH CA AH CB AH CG AH CD AH NE AH	SN 595 RG 596	52. 442 53. 421 54. 726 54. 550 53. 894 53. 398 54. 479 55. 467	71. 921 78. 688 77. 715 78. 378 79. 898 80. 426 81. 856 82. 760 83. 112 82. 635	44. 800 45. 824 44. 031 44. 171 44. 141 42. 880 43. 096 43. 482 42. 671 41. 431	1.00 22.25 1.00 22.44 1.00 22.52 1.00 21.28 1.00 21.31 1.00 22.01 1.00 20.88 1.00 21.35 1.00 22.62	A A A A A A A	O N C C C C N C

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					FIG. 4-95	(Continued)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	4606 4607 4608 4610 4611 4612 4613 4614 4615 4616 4621 4622 4623 4624 4625 4626 4627 4628 4629 4630 4631 4632 4633 4634 4635 4636 4637 4638 4639 4641 4642 4643 4644 4644 4644 4644 4644	C O N CA CB CCD CCD N CA CB CD N CA	THR THR THR PHE PHE PHE PHE PHE PHE	596 596 597 597 597 597 597 597 598 598 598 598 599 599 600 600 601 601 601 601	56. 427 83. 924 43. 096 1. 00 19. 92 A 55. 492 77. 982 45. 440 1. 00 21. 53 A 56. 482 78. 611 45. 804 1. 00 20. 59 A 55. 046 76. 930 46. 107 1. 00 21. 98 A 55. 705 76. 512 47. 331 1. 00 21. 98 A 54. 943 77. 061 48. 539 1. 00 23. 55 A 55. 184 78. 547 48. 776 1. 00 30. 86 A 56. 611 78. 813 49. 264 1. 00 30. 86 A 56. 891 80. 239 49. 414 1. 00 34. 81 A 57. 014 81. 088 48. 401 1. 00 36. 01 A 57. 326 82. 365 48. 650 1. 00 37. 36 A 55. 869 75. 011 47. 458 1. 00 20. 79 A 55. 523 74. 423 48. 487 1. 00 20. 79 A 56. 400 74. 398 46. 404 1. 00 19. 44 A 56. 649 72. 963 46. 387 1. 00 18. 20 A 56. 691 <	(Continued) N C O N C C C C N C N C C C C C C C C
ATOM ATOM ATOM ATOM	4645 4646 4647 4648	CE1 CE2 CZ C	PHE PHE PHE PHE	601 601 601 601	51.100 76.271 52.603 1.00 29.10 A 52.160 75.650 54.680 1.00 28.02 A 51.658 76.636 53.830 1.00 28.61 A 52.623 70.265 52.635 1.00 22.45 A	C C C C
ATOM ATOM ATOM ATOM ATOM ATOM	4649 4650 4651 4652 4653 4654	O N CA CB CG	PHE GLU GLU GLU GLU	601 602 602 602 602	52. 235 69. 451 53. 470 1. 00 22. 89 A 52. 884 69. 931 51. 374 1. 00 22. 76 A 52. 712 68. 556 50. 931 1. 00 21. 82 A 52. 956 68. 418 49. 422 1. 00 22. 43 A 54. 396 68. 559 48. 974 1. 00 27. 44 A	O N C C C
UIOM	TUUT	עט	GLU	602	54.872 70.002 48.893 1.00 29.71 A	С

					FΙ	G. 4	- 96			(Continued)
ATOM ATOM	4655		GLU GLU	602 602	54. 751	70. 743	49.891	1.00 31.66	A	0
ATOM	4656 4657	C	GLU	602	55. 379 53. 663	70. 392 67. 657	47. 822 51. 698	1.00 31.46 1.00 21.67	A	0
ATOM	4658	ŏ	GLU	602	53. 386	66. 473	51.899	1.00 22.33	A A	C 0
ATOM	4659	Ň	VAL	603	54.777	68. 229	52. 146	1.00 20.78	A	N
ATOM	4660	CA	VAL	603	55. 772	67. 468	52.897	1.00 20.76	Ä	Ċ
ATOM	4661	CB	VAL	603	57. 159	68.133	52.800	1.00 18.99	Ä	č
ATOM	4662	CG1	VAL	603	58. 165	67.365	53.649	1.00 15.00	A	Č
ATOM	4663	CG2	VAL	603	57.603	68.193	51.335	1.00 15.21	Α	С
ATOM	4664	C	VAL	603	55.368	67.350	54.364	1.00 21.85	Α	C
ATOM	4665	0	VAL	603	55. 373	66.265	54.946	1.00 20.44	Α	0
ATOM	4666	N	GLU	604	55.009	68. 481	54. 951	1.00 24.70	Α	N
ATOM	4667	CA	GLU	604	54. 594	68. 518	56. 341	1.00 27.84	Α	С
ATOM	4668	CB	GLU	604	54. 322	69.964	56.770	1.00 30.83	A	Ç
ATOM	4669	CG	GLU	604	55. 572	70.808	56. 924	1.00 37.92	A	C
ATOM ATOM	4670 4671	CD	GLU GLU	604	56.449	70. 355	58. 091	1.00 43.63	A	C
ATOM	4672		GLU	604 604	57. 505 56. 083	70. 989 69. 368	58. 328 58. 773	1.00 46.30	A	0
ATOM	4673	C	GLU	604	53. 349	67.669	56. 553	1.00 45.85 1.00 27.28	A	0
ATOM	4674	ŏ	GLU	604	53. 270	66.909	57. 517	1.00 21.28	A A	C 0
ATOM	4675	Ň	ASP	605	52. 381	67. 786	55.650	1.00 25.92	A	N N
ATOM	4676	CA	ASP	605	51. 151	67.021	55.785	1.00 25.72	A	Č
ATOM	4677	CB	ASP	605	50. 144	67. 436	54. 713	1.00 24.61	Ä	č
ATOM	4678	CG	ASP	605	49.576	68.832	54.963	1.00 23.36	Ä	č
ATOM	4679		ASP	605	48.677	69.267	54.215	1.00 23.15	Ā	Ŏ
ATOM	4680		ASP	605	50. 036	69.499	55.914	1.00 21.27	Α	0
ATOM	4681	C	ASP	605	51.379	65. 515	55. 783	1.00 26.18	Α	C
ATOM	4682	0	ASP	605	50.646	64. 779	56.439	1.00 28.35	A	0
ATOM	4683	N	GLN	606	52. 394	65. 051	55.063	1.00 26.16	Α	N
ATOM	4684	CA	GLN	606	52.704	63. 627	55.056	1.00 25.29	A	C
ATOM ATOM	4685	CB CG	GLN	606	53. 788	63. 302	54.026	1.00 24.18	A	C
ATOM	4686 4687	CD	GLN GLN	606 606	53. 305	63. 332	52. 596	1.00 24.92	A	C
ATOM	4688		GLN	606	52. 206 52. 373	62. 321 61. 122	52. 330 52. 560	1.00 24.81	A	C
ATOM	4689		GLN	606	51.075	62. 801	51.840	1.00 25.31 1.00 25.44	A	0 N
ATOM	4690	C	GLN	606	53. 207	63. 268	56.447	1.00 25.44	A A	N C
ATOM	4691	Ŏ	GLN	606	52. 838	62. 238	57.002	1.00 25.41	A	Ö
ATOM	4692	N	ILE	607	54. 059	64. 129	57.001	1.00 26.84	A	N
ATOM	4693	CA	ILE	607	54.607	63. 915	58. 337	1.00 28.30	A	C
ATOM	4694	CB	ILE	607	55. 639	65.002	58.702	1.00 28.21	Ä	č
ATOM	4695	CG2		607	56. 165	64.778	60.116	1.00 26.82	Ā	C C
ATOM	4696	CG1		607	56. 789	64. 977	57.694	1.00 29.86	Α	Ċ
ATOM	4697	CD1		607	57. 796	66.086	57.881	1.00 28.34	Α	C
ATOM	4698	C	ILE	607	53. 470	63.963	59. 355	1.00 29.50	Α	С
ATOM	4699	0	ILE	607	53. 359	63.093	60. 226	1.00 27.80	Α	0
ATOM	4700	N	GLU	608	52.619	64. 978	59. 239	1.00 30.32	A	Ŋ
ATOM ATOM	4701 4702	CA CB	GLU	608	51.508	65. 099	60.164	1.00 32.21	Ą	C
ATOM	4702		GLU GLU	608 608	50.705	66.379	59.919	1.00 33.05	A	C
VION	7100	UU	ԱՐՈ	UUO	49. 578	66. 581	60. 936	1.00 34.99	Α	C

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										(Continued)
					FΙ	G. 4	9 7			(00000000000000000000000000000000000000
ATOM	4704	CD	GLU	608	50.054	66. 482	62.389	1.00 38.42	·A	. C
ATOM	4705	OE1		608	49. 197	66.454	63.302	1.00 37.67	A	0
ATOM	4706		GLU	608	51. 285	66. 435	62.625	1.00 40.64	Α	0
ATOM	4707	C	GLU	608	50.606	63.891	60.012	1.00 32.76	Α	C
ATOM	4708	Ō	GLU	608	49.889	63.527	60.947	1.00 33.47	Α	0
ATOM	4709	N	ALA	609	50.643	63.270	58.836	1.00 31.32	Α	N
ATOM	4710	CA	ALA	609	49.827	62.090	58.595	1.00 30.73	Α	C
ATOM	4711	CB	ALA	609	49.883	61.682	57.123	1.00 28.50	Α	С
ATOM	4712	C	ALA	609	50. 355	60.968	59.472	1.00 30.16	Α	С
ATOM	4713	0	ALA	609	49. 583	60.274	60.139	1.00 31.03	Α	0
ATOM	4714	N	ALA	610	51.674	60.803	59.479	1.00 29.26	Α	N
ATOM	4715	CA	ALA	610	52.310	59. 758	60.274	1.00 28.48	Α	C
ATOM	4716	CB	ALA	610	53.826	59.818	60.114	1.00 27.67	A	C
ATOM	4717	C	ALA	610	51.930	59.886	61.743	1.00 27.62	A	C
ATOM	4718	0	ALA	610	51.556	58.904	62.379	1.00 28.43	A	0
ATOM	4719	N	ARG	611	52.025	61.094	62. 282	1.00 26.94	A	N
ATOM -	4720	CA	ARG	611	51.674	61.309	63.678	1.00 28.98	A	C
ATOM	4721	CB	ARG	611	51.812	62. 787	64.042	1.00 28.96	A	C
ATOM	4722	CG	ARG	611	53. 239	63. 291	64.032	1.00 29.26	A	C
ATOM	4723	CD	ARG	611	53. 281	64. 799	64.187	1.00 29.92	A	C
ATOM	4724	NE	ARG	611	54. 641	65.322	64. 102	1.00 28.90	A	N .
ATOM	4725	CZ	ARG	611	54. 980	66. 384		1.00 29.97	A	C
ATOM	4726		ARG	611	54.055	67. 028	62.680	1.00 31.41	A	Ň
ATOM	4727		ARG	611	56. 237	66.802	63. 347	1.00 29.57	A	N
ATOM	4728	C	ARG	611	50. 242	60.846	63. 923	1.00 29.90	A	C
ATOM	4729	0	ARG	611	49. 983	60.084	64.856	1.00 31.08	A	0
ATOM	4730	N	GLN	612	49.319	61.298 60.922	63. 076 63. 195	1.00 30.18 1.00 30.42	A A	N C
ATOM	4731	CA	GLN	612 612	47. 916 47. 108	61.497	62.035	1.00 30.42	A	C
ATOM	4732 4733	CB CG	GLN	612	47. 112	63.001	61.964	1.00 33.70	A	Č
ATOM	4734	CD	GLN GLN	612	46. 446	63.637	63. 162	1.00 34.91	A	Č
ATOM ATOM	4735		GLN	612	45. 276	63. 379	63.444	1.00 35.03	A	ŏ ·
ATOM	4736		GLN	612	47. 188	64. 475	63.875	1.00 35.30	Ä	Ň
ATOM	4737	C	GLN	. 612	47. 740	59.405	63. 223	1.00 30.70	Ä	Ĉ
ATOM	4738	ŏ	GLN	612	46. 993	58.878	64.049	1.00 31.56	Ä	Ö
ATOM	4739	Ň	PHE	613	48. 415	58.698	62.324	1.00 30.50	Ä	Ň
ATOM	4740	ĊA	PHE	613	48. 291	57. 248	62.301	1.00 32.33	Ä	Ċ
ATOM	4741	CB	PHE	613	49.043	56.653	61.114	1.00 31.37	A	
ATOM	4742	CG	PHE	613	48. 537	57. 126	59.787	1.00 30.49	A	Ċ
ATOM	4743		PHE	613	47. 167	57. 171	59.529	1.00 30.03	A	Ċ
ATOM	4744		PHE	613	49. 423	57.523	58.793	1.00 28.11	Α	С
ATOM	4745		PHE	613	46. 687	57.604	58.300	1.00 29.96	A	C C C C
ATOM	4746		PHE	613	48. 954	57.959	57.559	1.00 28.75	Α	C
ATOM	4747	CZ	PHE	613	47. 585	58.001	57.309	1.00 28.70	Α	C
ATOM	4748	C	PHE	613	48.835	56.679	63.597	1.00 34.28	Α	C
ATOM	4749	0	PHE	613	48.327	55.677	64.107	1.00 34.47	Α	0
ATOM	4750	N	SER	614	49.865	57.326	64.134	1.00 35.61	Α	N
ATOM	4751	CA	SER	614	50.454	56.884	65.388	1.00 37.88	A	C
ATOM	4752	CB	SER	614	51.723	57. 677	65.683	1.00 38.32	A	C

						(Continued)
				FIG. 4-98		(001102114104)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	4753 OG 4754 C 4755 O 4756 N 4757 CA 4758 CB 4759 CG 4760 CD 4761 CE 4762 NZ 4763 C 4764 O 4765 N 4766 CA 4767 CB 4768 CG	MET MET	614 614 615 615 615 615 615 615 616 616 616	52. 686 57. 477 64. 663 1. 00 49. 424 57. 098 66. 494 1. 00 49. 283 56. 276 67. 398 1. 00 48. 694 58. 204 66. 413 1. 00 47. 663 58. 490 67. 400 1. 00 47. 047 59. 870 67. 155 1. 00 47. 084 61. 040 67. 642 1. 00 47. 064 62. 330 67. 631 1. 00 47. 864 63. 511 68. 168 1. 00 48. 314 63. 301 69. 577 1. 00 45. 794 57. 285 68. 303 1. 00 45. 418 55. 712 66. 065 1. 00 45. 246 55. 374 64. 578 1. 00 45. 673 56. 532 63. 768 1. 00	O 38. 53 A O 39. 76 A O 41. 47 A O 40. 51 A O 41. 32 A O 42. 73 A O 44. 59 A O 46. 18 A O 46. 73 A O 48. 03 A O 40. 86 A O 41. 94 A O 39. 78 A O 37. 88 A O 37. 88 A O 37. 42 A O 35. 95 A	(Continued) 0 C 0 N C C C C C C C C C C C C C C C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	4769 SD 4770 CE 4771 C 4772 0 4773 N 4774 CA 4775 C 4776 0 4777 N 4778 CA	MET MET MET GLY GLY GLY GLY PHE PHE	616 616 616 617 617 617 617 618 618	44. 195 56. 101 62. 079 1. 00 43. 946 57. 730 61. 385 1. 00 45. 654 54. 447 66. 885 1. 00 44. 908 53. 473 66. 772 1. 00 46. 706 54. 469 67. 698 1. 00 47. 013 53. 355 68. 578 1. 00 47. 445 51. 995 68. 065 1. 00 47. 806 51. 143 68. 872 1. 00 47. 409 51. 751 66. 761 1. 00 47. 841 50. 447 66. 262 1. 00	0 35. 73 A 0 34. 06 A 0 36. 90 A 0 37. 22 A 0 35. 15 A 0 32. 74 A 0 32. 72 A 0 33. 71 A 0 32. 52 A 0 31. 36 A	S C O N C C O N C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	4782 CD 4783 CE	PHE PHE PHE PHE PHE VAL VAL	618 618 618 618 618 618 618 618 619 619	46. 047 50. 624 64. 457 1. 0 46. 743 51. 025 63. 322 1. 0 44. 724 51. 027 64. 607 1. 0 46. 129 51. 815 62. 349 1. 0 44. 104 51. 814 63. 642 1. 0 44. 808 52. 209 62. 509 1. 0 49. 109 50. 521 65. 404 1. 0 49. 303 49. 735 64. 477 1. 0 49. 982 51. 465 65. 732 1. 0 51. 226 51. 627 64. 996 1. 0	0 31. 10 A 0 31. 61 A 0 31. 30 A 0 30. 93 A 0 31. 53 A 0 30. 94 A 0 29. 86 A 0 30. 95 A 0 30. 95 A 0 30. 23 A 0 29. 99 A 0 29. 39 A	C C C C C C O N C C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	4791 CG 4792 CG 4793 C 4794 O 4795 N 4796 CA 4797 CB 4798 CG 4799 OD	1 VAL 2 VAL VAL VAL ASP ASP ASP	619 619 619 619 620 620 620 620 620	52. 632 53. 200 63. 617 1. 0 50. 248 52. 804 62. 994 1. 0 52. 425 51. 673 65. 931 1. 0 52. 400 52. 342 66. 962 1. 0 53. 475 50. 954 65. 561 1. 0 54. 695 50. 932 66. 347 1. 0 55. 563 49. 748 65. 924 1. 0 56. 789 49. 587 66. 794 1. 0 57. 191 50. 580 67. 439 1. 0 57. 358 48. 473 66. 818 1. 0	0 28.74 A 0 26.48 A 0 29.66 A 0 30.05 A 0 29.84 A 0 29.07 A 0 27.94 A 0 27.02 A 0 26.38 A 0 25.22 A 0 30.30 A	C C O N C C C O O C

			(Continued)						
ATOM ATOM ATOM	4802 4803 4804	N CA	ASP 62 ASN 62 ASN 62	0 56. 009 1 55. 330 1 55. 962	53. 196 54. 492	64. 979 66. 958 66. 746	1.00 29.95 1.00 33.01 1.00 35.15	A A A	0 N C
ATOM ATOM ATOM	4805 4806 4807			1 56. 420 1 57. 648	54.804	67. 975 69. 214 69. 346	1.00 38.29 1.00 43.03 1.00 44.79	A A A	C C O
ATOM ATOM ATOM	4808 4809 4810		ASN 62 ASN 62 ASN 62	1 57. 453	3 54.370	70. 130 66. 441 66. 004	1.00 45.61 1.00 35.20 1.00 34.67	A A A	N C O
ATOM ATOM ATOM	4811 4812 4813	N I CA I	LYS 62 LYS 62 LYS 62	2 58. 016 2 59. 439	5 53.186 5 52.977	66. 660 66. 418 67. 464	1.00 36.30 1.00 35.70 1.00 37.42	A A A	N C C
ATOM ATOM ATOM	4814 4815 4816	CG I	LYS 62 LYS 62 LYS 62 LYS 62	2 60.148 2 60.763	52.611 51.584	68. 866 69. 804 71. 240	1. 00 39. 14 1. 00 43. 05 1. 00 45. 27	A A A	C C C
ATOM ATOM ATOM	4817 4818 4819	NZ I C I	LYS 62 LYS 62 LYS 62	2 61.516 2 59.762	51.077 52.445	72. 123 65. 036 64. 571	1. 00 45. 73 1. 00 34. 38 1. 00 35. 67	A A A	N C O
ATOM ATOM ATOM	4820 4821 4822	N A	ARG 62 ARG 62 ARG 62	3 58. 783 3 59. 030	51.846 51.308	64. 374 63. 046 63. 058	1. 00 31. 86 1. 00 29. 60 1. 00 29. 94	A A A	N C C
ATOM ATOM ATOM	4823 4824 4825	CG A	ARG 62 ARG 62 ARG 62	3 59.767 3 59.117	49. 071 47. 832	64. 009 64. 614 63. 758	1. 00 32. 12 1. 00 33. 42 1. 00 34. 25	A A A	C C N
ATOM ATOM ATOM	4826 4827 4828		ARG 62 ARG 62	3 58. 457 3 57. 476	45. 601 45. 572	63. 833 64. 725 63. 021	1. 00 34. 36 1. 00 35. 41 1. 00 33. 15	A A A	C N N
ATOM ATOM ATOM	4829 4830 4831	C A O A	ARG 62 ARG 62 ILE 62	3 58. 179 3 57. 315	51.957 51.313	61.962 61.363 61.720	1. 00 27. 66 1. 00 27. 44 1. 00 25. 16	A A A	C O - N
ATOM ATOM ATOM	4832 4833 4834	CA]	ILE 62-	4 57. 708 4 57. 114	53. 977 55. 298	60. 685 61. 224 60. 107	1.00 24.70 1.00 24.52 1.00 23.47	A A A	C C C
ATOM ATOM ATOM	4835 4836 4837	CG1 I	ILE 62	4 56. 136 4 55. 473	55. 021 56. 277	62. 371 62. 936 59. 532	1.00 24.01 1.00 19.15 1.00 24.37	A A	C C C
ATOM ATOM ATOM	4838 4839 4840	0 I N A	ILE 624 NLA 625 NLA 625	59.651 58.384	55. 034 53. 768	59. 709 58. 356 57. 189	1.00 23.38 1.00 22.58	A A A	0 N
ATOM ATOM ATOM	4841 4842 4843	CB A	NLA 62: NLA 62: NLA 62: NLA 62:	59.650 58.430	52. 693 54. 833	56. 579 56. 168 56. 275	1.00 21.00 1.00 20.21 1.00 21.28	A A A	C C
ATOM ATOM ATOM	4844 4845 4846	N I CA I	LE 626 LE 626 LE 626	5 59. 135 5 58. 502	55. 385 56. 178	55. 185 54. 137	1.00 21.90 1.00 19.63 1.00 18.63	A A A	O N C
ATOM ATOM	4847 4848	CG2 I	LE 626 LE 626	60. 032 57. 973	58. 103 58. 501	54. 446 54. 694 53. 296	1.00 18.98 1.00 18.36 1.00 19.11	A A A	C C
ATOM ATOM	4849 4850	CD1 I	LE 626 LE 626		59. 991 55. 882	53. 562 52. 809	1.00 18.34 1.00 17.48	A A	C

										(Cont	inued)
					FIC	3. 4 -	100			COH	inaca
										•	
ATOM			ILE	626	60. 380	55.619	52.776	1.00 17.10 1.00 17.62	A	O N	
ATOM			TRP	627	58. 425	55. 893	51.719	1.00 17.02	A A	C	
ATOM	4853		TRP	627	58. 998	55.622	50. 409 50. 206	1.00 17.02	A		
ATOM	4854		TRP	627	59. 190	54.118	49. 427	1.00 10.00	A	C C	
ATOM	4855		TRP	627	58.096	53. 441		1.00 18.70	A	Č	
ATOM	4856		TRP	627	58. 139	53.055	48. 044 47. 749	1.00 17.30	A	č	
ATOM	4857	CE2		627	56. 912	52. 425	47. 028	1.00 17.10	A	č	
ATOM	4858	CE3		627	59.095	53. 179	49. 895	1.00 13.10	A	č	
ATOM	4859		TRP	627	56.879	53.047	48. 896	1.00 18.72	A	N	
ATOM	4860		TRP	627	56. 163	52. 435 51. 916	46. 480	1.00 16.42	A	Ċ	
ATOM	4861		TRP	627	56.617	52. 673	45. 769	1.00 10.42	A	Č	
ATOM	4862		TRP	627	58. 801 57. 575	52.013	45. 507	1.00 14.40	Ä	Č	
ATOM	4863		TRP	627	58. 157	56. 191	49. 275	1.00 18.48	Ä	č	
ATOM	4864	C	TRP	627 627	56. 934	56. 280	49. 381	1.00 18.15	Ä	Ŏ	
ATOM	4865	0	TRP	628	58. 829		48. 193	1.00 18.70	Ā	N	
ATOM	4866	N	GLY GLY	628	58. 140	57.146	47. 049	1.00 18.30	Ā	Ċ	
ATOM	4867	CA	GLY	628	58. 986	57. 163	45. 787	1.00 18.36	Ā	Č	
ATOM	4868	C 0	GLY	628	60. 212		45. 833	1.00 19.07	A	0	
ATOM	4869	N	TRP	629	58. 312		44. 654	1.00 17.25	Ā	N	
ATOM	4870 4871	CA	TRP	629	58. 945	57. 322	43. 343	1.00 15.27	A	C	
ATOM ATOM	4872	CB	TRP	629	EO 30E		42. 494	1.00 10.48	A	С	
ATOM	4873	CG	TRP	629	59. 131	55. 698	41. 357	1.00 10.84	Α	С	
ATOM	4874		TRP	629	59. 512		41. 122	1.00 9.02	Α	С	
ATOM	4875		TRP	629	60. 243		39. 914	1.00 10.87	Α	C	
ATOM	4876		TRP	629	59. 312		41.818	1.00 9.31	Α	С	
ATOM	4877		TRP	629	59. 635		40.313	1.00 10.72	Α	С	
ATOM	4878		TRP	629	60. 299		39. 443	1.00 10.74	A	N	
ATOM	4879		TRP	629	60.779		39. 379	1.00 12.40	Α	C	
ATOM	4880		TRP	629	59.842		41.295	1.00 11.95	Α	C C	
ATOM	4881		TRP	629	60.571		40.080	1.00 13.29	Α	С	
MOTA	4882	C	TRP	629	58.671		42.753	1.00 15.91	Α	Č	
MOTA	4883	Ö	TRP	629	57.622			1.00 15.58	A	0	
ATOM	4884	N	SER	630	59.612	59. 269		1.00 16.99	A	N	
ATOM	4885	CA	SER	630	59. 453	60.603		1.00 16.78	A	C	
MOTA	4886	CB	SER	630	58. 258			1.00 18.65	A	C	
ATOM	4887	0G	SER	630	58. 531			1.00 22.38	A	0	
ATOM	4888	С	SER	630	59. 234			1.00 16.69	A	C	
ATOM	4889	0	SER	630	60.076			1.00 17.90	A	0	
ATOM	4890	N	TYR	631	58. 093			1.00 17.21	A	N	
ATOM	4891	CA	TYR	631	57. 737			1.00 15.51	A	C	
ATOM	4892	CB	TYR	631	56.380			1.00 17.16	A	C	
ATOM	4893	CG	TYR	631	56.161			1.00 18.38	A	C	
ATOM	4894	CD1			55. 947			1.00 18.79	A	C	
ATOM	4895		TYR		55. 741			1.00 19.48	A	C C	
ATOM	4896		TYR		56. 168				A	C	
MOTA	4897		YYR		55. 963			1.00 19.30	A A	C	
MOTA	4898		TYR		55. 748				A A	Õ	
MOTA	4899	OH	TYR	631	55. 520	69.173	45.084	1.00 20.71	А	U	

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(Continued)											
					FIC	3. 4 -	101				
ATOM ATOM	4900 4901	C 0	TYR TYR	631 631	57. 672 57. 946	62. 632 63. 201	44. 668 45. 731	1.00 15.27 1.00 13.23	A A	C 0	
ATOM	4902	N CA	GLY	632	57. 324	61.350	44. 592	1.00 14.83	A	N C	
ATOM ATOM	4903 4904	CA C	GLY GLY	632 632	57. 266 58. 653	60. 529 60. 477	45. 783 46. 394	1.00 15.04 1.00 14.53	A A	C C	
ATOM	4905	Ŏ	GLY	632	58. 816	60.652	47. 596	1.00 13.85	Ä	Ŏ	
ATOM	4906	N	GLY	633	59.655	60. 246	45. 551	1.00 15.63	A	N	
ATOM	4907	CA	GLY	633	61.030	60. 185	46.014	1.00 14.69	A	C	
ATOM ATOM	4908 4909	C 0	GLY GLY	633 633	61.500 62.251	61.513 61.561	46. 576 47. 555	1.00 15.25 1.00 16.82	A A	C 0	
ATOM	4910	Ň	TYR	634	61.058	62. 598	45. 954	1.00 13.67	A	N	
ATOM	4911	CA	TYR	634	61.418	63.940	46.398	1.00 13.29	A	Ċ	
ATOM	4912	CB	TYR	634	60. 901	64.964	45. 397	1.00 11.67	A	C	
ATOM	4913	CC	TYR TYR	634	60.914	66. 382	45.904	1.00 12.54	A	C	
ATOM ATOM	4914 4915		TYR	634 634	62. 112 62. 125	67. 069 68. 398	46. 072 46. 484	1.00 13.46 1.00 13.37	A A	C C	
ATOM	4916		TYR	634	59. 723	67.057	46. 173	1.00 11.38	A	Č	
ATOM	4917		TYR	634	59. 727	68. 383	46.586	1.00 11.86	Ā	Č	
ATOM	4918	CZ	TYR	634	60. 933	69.049	46. 734	1.00 12.83	A	C	
ATOM	4919	OH C	TYR	634	60.957	70.375	47. 091	1.00 12.97	A	0	
ATOM ATOM	4920 4921	C 0	TYR TYR	634 634	60.829 61.524	64. 240 64. 721	47. 778 48. 672	1.00 14.36 1.00 16.28	A A	C 0	
ATOM	4922	N	VAL	635	59. 542	63. 968	47. 949	1.00 10.28	A	N N	
ATOM	4923	CA	VAL	635	58.899	64. 218	49. 231	1.00 15.44	Ä	Ċ	
ATOM	4924	CB	VAL	635	57. 364	64.025	49.135	1.00 15.15	Α	C	
ATOM	4925		VAL	635	56. 743	63. 988	50. 524	1.00 14.56	A	C	
ATOM ATOM	4926 4927	C	VAL VAL	635 635	56. 758 59. 486	65. 167 63. 296	48. 326 50. 294	1.00 12.62 1.00 16.48	. A	C	
ATOM	4928	Ö	VAL	635	59. 681	63. 711	50. 234	1.00 16.48	A A	C 0	
ATOM	4929	Ň	THR	636	59. 779	62.054	49. 917	1.00 16.16	A	Ň	
ATOM	4930	CA	THR	636	60.368	61.098	50.855	1.00 18.40	A	Ċ	
ATOM	4931	CB	THR	636	60. 701	59. 746	50. 175	1.00 18.30	Α	C	
ATOM ATOM	4932 4933	0G1		636	59.504	59. 130	49.696	1.00 20.57	A	0	
ATOM	4933	CGZ	THR THR	636 636	61.362 61.676	58. 807 61. 676	51. 157 51. 396	1.00 20.48 1.00 19.91	A A	C C	
ATOM	4935	ŏ	THR	636	61.914	61.696	52. 609	1.00 19.58	A	Ö	
ATOM	4936	N	SER	637	62.524	62.141	50. 483	1.00 19.89	A	Ň	
ATOM	4937	CA	SER	637	63. 804	62.711	50.862	1.00 20.30	Α	C	
ATOM	4938	CB	SER	637	64. 599	63. 086	49.614	1.00 19.17	A	C	
ATOM ATOM	4939 4940	OG C	SER SER	637 637	64. 823 63. 615	61.952	48. 800	1.00 19.07	. A	0	
ATOM	4941	Ô	SER	637	64. 235	63. 938 64. 049	51. 749 52. 812	1.00 21.61 1.00 22.54	A A	C . 0	
ATOM	4942	N	MET	638	62. 760	64. 855	51. 309	1.00 22.04	A	N N	
ATOM	4943	CA	MET	638	62.490	66.074	52.066	1.00 21.87	Ä	Ċ	
ATOM	4944	CB	MET	638	61.417	66.895	51.354	1.00 20.36	Α	C	
ATOM	4945	CC	MET	638	61.876	67.465	50.032	1.00 21.23	A	С	
ATOM ATOM	4946 4947	SD CE	MET MET	638 638	63. 069 62. 006	68. 787 70. 229	50. 261 50. 125	1.00 21.33 1.00 19.31	A A	S C	
ATOM	4948	C	MET	638	62.039	65. 748	53. 494	1.00 19.51	A	C	

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					FIC	G. 4-	102			(Continued)
ATOM	4949	0	MET	638	62. 511	66. 351	54. 472	1.00 19.64	Α	0	
ATOM	4950	N	VAL	639	61.116	64. 798	53.600	1.00 19.63	Α	N	
ATOM	4951	CA	VAL	639	60.611		54. 891	1.00 20.04	Α	C	
ATOM	4952	CB	VAL	639	59. 524		54. 746	1.00 20.08	Α	С	
ATOM	4953	CG1	VAL	639	59. 201	62.688	56. 112	1.00 20.55	Α	С	
ATOM	4954	CG2	VAL	639	58. 275		54. 108	1.00 17.95	Α	С	
ATOM	4955	C	VAL	639	61.758		55. 692	1.00 20.25	Α	C	
ATOM	4956	0	VAL	639	61.986		56. 831	1.00 23.11	A	0	
ATOM	4957	N	LEU	640	62. 489		55. 088	1.00 20.83	A	N	
ATOM	4958	CA	LEU	640	63.608		55. 765	1.00 22.08	A	C	
ATOM	4959	CB	LEU	640	64. 245	61.179	54. 855	1.00 22.31	A	C	
ATOM	4960		LEU	640	63. 400		54. 570	1.00 21.31	A	C	
ATOM	4961		LEU	640	64. 143		53.611	1.00 22.16	A	C	
ATOM	4962		LEU	640	63. 105	59. 205	55. 863	1.00 22.25 1.00 23.38	A	C C	
ATOM ATOM	4963 4964	C	LEU LEU	640 640	64. 675 65. 416	63. 212 62. 922	56. 239 57. 182	1.00 23.38	A	0	
ATOM	4965	O N	GLY	641	64. 745	64. 374	55. 592	1.00 22.33	A A	N N	
ATOM	4966	CA	GLY	641	65. 731	65. 368	55. 972	1.00 23.10	A	C	
ATOM	4967	C	GLY	641	65. 153	66. 555	56. 721	1.00 23.73	Ä	Č	
ATOM	4968	ŏ	GLY	641	65. 782	67. 609	56. 802	1.00 23.94	A	ŏ	
ATOM	4969	Ň	SER	642	63. 958		57. 278	1.00 22.74	Ä	Ň	
ATOM	4970	CA	SER	642	63. 318	67.484	58.002	1.00 20.76	A	Ċ	
ATOM	4971	CB	SER	642	61.798	67.370	57.883	1.00 19.77	Ä	Č	
ATOM	4972	0G	SER	642	61.319	66.213	58.546	1.00 17.97	A	0	
ATOM	4973	C	SER	642	63. 723	67.488	59.471	1.00 21.73	Α	С	
ATOM	4974	0	SER	642	63. 656	68.519	60.140	1.00 21.40	Α	0	
ATOM	4975	N	GLY	643	64. 136	66.327	59.967	1.00 22.24	Α	N	
ATOM	4976	CA	GLY	643	64. 548	66. 213	61.350	1.00 22.64	A	C	
ATOM	4977	C	GLY	643	63. 407	65.944	62.314	1.00 23.74	A	C	
ATOM	4978	0	GLY	643	63. 585	66.064	63. 528	1. 00 25. 32	A	0	
ATOM	4979	N	SER	644	62. 244	65. 573	61.786	1.00 23.53	A	N	
ATOM	4980	CA	SER	644	61.067	65. 301	62.616	1.00 23.38	A	C	
ATOM	4981 4982	CB	SER SER	644	59. 850	64. 995	61.742	1.00 24.79	A	C	
ATOM ATOM	4983	OG C	SER	644 644	59. 898 61. 287	63. 666 64. 129	61.247 63.559	1. 00 24. 45 1. 00 23. 18	A	0 C	
ATOM	4984	Ö	SER	644	60. 565	63. 961	64. 536	1.00 23.18	A A	0	
ATOM	4985		GLY			63. 307		1. 00 24. 26	Ä	N	
ATOM	4986	CA	GLY	645	62. 543	62. 166	64.107	1.00 24.80	A	Č	
ATOM	4987	C	GLY	645	61. 398	61.175	64. 114	1.00 24.80	A	Č	
ATOM	4988	Ŏ	GLY	645	61.379	60. 248	64. 920	1.00 27.93	Ä	ŏ	
ATOM	4989	Ň	VAL	646	60. 446	61.357	63. 207	1.00 23.98	Ä	Ň	
ATOM	4990	CA	VAL	646	59. 289	60.474	63. 121	1.00 22.32	Ä	Ċ	
ATOM	4991	CB	VAL	646	58. 092	61.207	62.473	1.00-24.36	Ä	Č	
ATOM	4992		VAL	646	56. 945	60.230	62. 215	1.00 22.37	Α	C	
ATOM	4993	CG2		646	57.636	62. 351	63.381	1.00 24.11	Α	С	
ATOM	4994	C	VAL	646	59. 552	59. 202	62.327	1.00 21.28	A	С	
ATOM	4995	0	VAL	646	59.079	58. 128	62.690	1.00 21.25	A	0	
ATOM	4996	N	PHE	647	60. 303	59. 326	61. 239	1.00 21.00	A	N	
ATOM	4997	CA	PHE	647	60. 593	58. 182	60. 380	1.00 18.33	A	С	

				FIG. 4-103	(Continued)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	5006 5007 5008 5009 5010 5011 5012 5013 5014 5015 5016 5017 5018 5019 5020 5021 5022 5023 5024	CB PHE CG PHE CD1 PHE CD2 PHE CE1 PHE CZ PHE C P	647 647 647 647 647 647 647 648 648 648 648 648 648 649 649 649 650 650 650	60. 497 58. 615 58. 924 1. 00 15. 79 59. 142 59. 131 58. 551 1. 00 16. 11 58. 138 58. 258 58. 152 1. 00 15. 39 58. 841 60. 479 58. 680 1. 00 14. 43 56. 855 58. 722 57. 894 1. 00 13. 82 57. 562 60. 943 58. 423 1. 00 15. 28 56. 568 60. 061 58. 031 1. 00 13. 75 61. 944 57. 555 60. 663 1. 00 18. 46 62. 943 58. 250 60. 825 1. 00 20. 84 61. 958 56. 232 60. 722 1. 00 17. 11 63. 165 55. 480 60. 996 1. 00 19. 06 62. 789 54. 105 61. 545 1. 00 17. 86 63. 961 53. 242 61. 955 1. 00 17. 94 63. 484 51. 869 62. 405 1. 00 19. 57 64. 594 51. 083 63. 095 1. 00 19. 22 65. 757 50. 894 62. 204 1. 00 20. 59 64. 025 55. 314 59. 747 1. 00 21. 47 65. 251 55. 379 59. 815 1. 00 23. 13 63. 376 55. 094 58. 610 1. 00 22. 38 64. 077 54. 898 57. 353 1. 00 24. 23 63. 156 55. 237 56. 181 1. 00 24. 09 61. 939 55. 319 56. 342 1. 00 27. 68 63. 130 52. 287 57. 313 1. 00 27. 68 63. 746 55. 426 55. 004 1. 00 21. 50 64. 961 55. 757 53. 834 1. 00 21. 50 62. 961 55. 757 53. 834 1. 00 21. 50 63. 649 55. 384 52. 535 1. 00 21. 13	CCCCCCCONCCCCNCONCCOSNCC
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	5026 5027 5028 5029 5030 5031 5032 5033 5034 5035 5036 5037 5038 5039 5040 5041 5042) VAL	650 651 651 651 651 651 651 652 652 652 652 653 653 653 653 654	64. 874 55. 333 52. 474 1. 00 21. 62 A 62. 857 55. 124 51. 499 1. 00 19. 35 A 63. 388 54. 753 50. 195 1. 00 19. 18 A 62. 896 53. 352 49. 758 1. 00 19. 03 A 63. 601 52. 933 48. 481 1. 00 17. 31 A 63. 173 52. 326 50. 853 1. 00 19. 60 A 62. 827 50. 901 50. 456 1. 00 18. 48 A 62. 953 55. 749 49. 120 1. 00 19. 53 A 61. 758 56. 015 48. 949 1. 00 19. 77 A 63. 925 56. 292 48. 393 1. 00 19. 77 A 63. 633 57. 240 47. 324 1. 00 15. 69 A 64. 323 58. 574 47. 594 1. 00 14. 98 A 64. 107 56. 662 45. 996 1. 00 14. 98 A 65. 288 56. 367 45. 827 1. 00 14. 68 A 63. 492 55. 963 43. 738 1. 00 14. 84 A 62. 805 <	O N C C C C C C C C C C C C C C C C C O N C C C C

						(Continued)
					FIG. 4-104	
ATOM	5047	CA	ALA	654	64. 289 58. 327 40. 845 1. 00 10.	68 A C
ATOM	5048	CB	ALA	654		27 A C
ATOM	5049	C	ALA	654	63.653 59.607 41.352 1.00 10.	
ATOM	5050	0	ALA	654	62. 687 60. 103 40. 787 1. 00 13.	
ATOM	5051	N	PRO	655	64. 208 60. 179 42. 420 1. 00 10.	
ATOM	5052	CD	PRO	655		01 A C
ATOM	5053	CA	PRO	655	63. 643 61. 408 42. 971 1. 00 10.	
ATOM ATOM	5054 5055	CB CG	PRO PRO	655 655		50 A C 23 A C
ATOM	5056	C	PRO	655	64. 090 62. 714 42. 327 1. 00 12.	
ATOM	5057	Ö	PRO	655	65.166 62.793 41.717 1.00 13.	
ATOM	5058	Ň	VAL	656	63. 245 63. 735 42. 454 1. 00 12.	
ATOM	5059	CA	VAL	656	63.612 65.065 41.999 1.00 12.	
ATOM	5060	CB	VAL	656	62. 373 65. 946 41. 769 1. 00 11.	42 A C
ATOM	5061	CG1		656	62. 781 67. 416 41. 645 1. 00 10.	
ATOM	5062		VAL	656	61. 661 65. 500 40. 510 1. 00 10.	
ATOM	5063	C	VAL	656	64. 382 65. 560 43. 236 1. 00 13.	
ATOM	5064	0	VAL	656	64. 038 65. 188 44. 355 1. 00 14.	
ATOM ATOM	5065 5066	N CA	SER SER	657 657	65. 419 66. 372 43. 066 1. 00 14. 66. 174 66. 831 44. 238 1. 00 14.	
ATOM	5067	CB	SER	657	67. 589 66. 231 44. 231 1. 00 15.	
ATOM	5068	OG	SER	657	68. 385 66. 819 43. 213 1. 00 15.	
ATOM	5069	C	SER	657	66. 286 68. 343 44. 320 1. 00 14.	
ATOM	5070	0	SER	657	66. 387 68. 912 45. 406 1. 00 14.	
ATOM	5071	N	ARG	658	66. 269 68. 978 43. 158 1. 00 15.	
ATOM	5072	CA	ARG	658	66. 388 70. 423 43. 038 1. 00 16.	
ATOM	5073	CB	ARG	658	67. 845 70. 787 42. 747 1. 00 20.	
ATOM	5074	CG	ARG	658	68. 142 72. 274 42. 582 1. 00 24.	
ATOM	5075	CD	ARG	658	69. 543 72. 450 42. 025 1. 00 25.	
ATOM ATOM	5076 5077	NE CZ	ARG ARG	658 658	69. 905 73. 838 41. 757 1. 00 25. 70. 353 74. 683 42. 676 1. 00 28.	
ATOM	5078	NH1	ARG	658	70. 491 74. 288 43. 935 1. 00 28.	
ATOM	5079		ARG	658	70. 690 75. 916 42. 329 1. 00 29.	
ATOM	5080	C	ARG	658	65. 515 70. 775 41. 850 1. 00 15.	
ATOM	5081	Ō	ARG	658	65. 752 70. 288 40. 735 1. 00 16.	
ATOM	5082	N	TRP	659	64.514 71.616 42.073 1.00 13.	
ATOM	5083	CA	TRP	659	63.603 71.967 40.999 1.00 13.	
ATOM	5084	CB	TRP	659	62. 465 72. 823 41. 550 1. 00 13.	
ATOM	5085	CG	TRP	659	61. 504 71. 963 42. 341 1. 00 17.	
ATOM	5086		TRP	659	60.690 70.898 41.829 1.00 16.	
ATOM	5087		TRP	659	60.027 70.313 42.927 1.00 18.	
ATOM ATOM	5088 5089		TRP TRP	659 659	60. 460 70. 382 40. 547 1. 00 16. 61. 300 71. 980 43. 692 1. 00 17.	
ATOM	5090	NE1		659	60.418 70.993 44.050 1.00 17.	
ATOM	5091		TRP	659	59. 145 69. 233 42. 785 1. 00 21.	
ATOM	5092	CZ3		659	59.584 69.311 40.403 1.00 18.	
ATOM	5093	CH2	TRP	659	58. 937 68. 746 41. 516 1. 00 20.	15 A C
MOTA	5094	C	TRP	659	64. 219 72. 580 39. 748 1. 00 13.	
ATOM	5095	0	TRP	659	63. 643 72. 503 38. 670 1. 00 11.	17 A O

				FIG. 4-105	(Co	ntinued)
ATOM	F00 <i>c</i>	N OU	660			
ATOM ATOM	5096 5097	N GLU CA GLU	660 660	65. 400 73. 163 39. 871 1. 00 14. 12 66. 042 73. 725 38. 697 1. 00 15. 96	A N A C	
ATOM	5098	CB GLU	660	67. 147 74. 704 39. 108 1. 00 16. 83	A C	
ATOM	5099	CG GLU	660	66. 548 76. 001 39. 626 1. 00 19. 65	A Č	
ATOM	5100	CD GLU	660	67.535 76.901 40.313 1.00 22.71	A C	
ATOM	5101	OE1 GLU	660	68.310 77.600 39.617 1.00 25.18	A 0	
ATOM	5102	OE2 GLU	660	67. 527 76. 907 41. 561 1. 00 23. 59	A 0	
ATOM ATOM	5103 5104	C GLU O GLU	660 660	66. 577 72. 635 37. 777 1. 00 15. 29 67. 001 72. 922 36. 659 1. 00 16. 67	A C	
ATOM	5105	N TYR	661	67. 001 72. 922 36. 659 1. 00 16. 67 66. 539 71. 383 38. 233 1. 00 14. 54	A O A N	
ATOM	5106	CA TYR	661	67. 003 70. 269 37. 399 1. 00 14. 57	A C	
ATOM	5107	CB TYR	661	67. 642 69. 154 38. 230 1. 00 13. 59	A C	
ATOM	5108	CG TYR	661	68. 878 69. 504 39. 035 1. 00 15. 73	A C	
ATOM	5109	CD1 TYR	661	69. 743 70. 531 38. 655 1. 00 13. 37	A C	
ATOM ATOM	5110	CE1 TYR CD2 TYR	661	70. 889 70. 805 39. 390 1. 00 12. 74	A C	
ATOM	5111 5112	CE2 TYR	661 661	69.199 68.765 40.166 1.00 16.63 70.338 69.027 40.898 1.00 16.03	A C	
ATOM	5113	CZ TYR	661	70. 338 69. 027 40. 898 1. 00 16. 03 71. 183 70. 041 40. 515 1. 00 13. 47	A C A C	
ATOM	5114	OH TYR	661	72.322 70.252 41.267 1.00 8.43	A O	
ATOM	5115	C TYR	661	65. 842 69. 637 36. 608 1. 00 15. 74	A C	
ATOM	5116	0 TYR	661	66.077 68.854 35.675 1.00 13.97	A 0	
ATOM ATOM	5117 5118	N TYR CA TYR	662	64.602 69.963 36.984 1.00 13.28	A N	
ATOM	5119	CB TYR	662 662	63. 445 69. 390 36. 308 1. 00 13. 00 62. 305 69. 143 37. 308 1. 00 14. 01	A C	
ATOM	5120	CG TYR	662	62. 305 69. 143 37. 308 1. 00 14. 01 61. 395 68. 026 36. 862 1. 00 14. 50	A C	
ATOM	5121	CD1 TYR	662	60.010 68.199 36.802 1.00 15.74	A C	
ATOM	5122	CE1 TYR	662	59. 184 67. 201 36. 273 1. 00 14. 99	Ä Č	
ATOM	5123	CD2 TYR	662	61. 930 66. 825 36. 400 1. 00 14. 83	A C	
ATOM ATOM	5124 5125	CE2 TYR CZ TYR	662	61. 122 65. 830 35. 873 1. 00 15. 13	A C	
ATOM	5126	OH TYR	662 662	59. 756 66. 024 35. 804 1. 00 15. 11 58. 983 65. 060 35. 214 1. 00 17. 05	A C	
ATOM	5127	C TYR	662	58. 983 65. 060 35. 214 1. 00 17. 05 62. 964 70. 251 35. 135 1. 00 12. 46	A O A C	
ATOM	5128	0 TYR	662	63. 320 71. 423 35. 030 1. 00 12. 22	A O	
ATOM	5129	N ASP	663	62.147 69.673 34.260 1.00 12.09	A N	
ATOM	5130	CA ASP	663	61. 686 70. 394 33. 076 1. 00 13. 20	A C	
ATOM ATOM	5131 5132	CB ASP CG ASP	663	60. 998 69. 427 32. 099 1. 00 11. 88	A C	
ATOM	5133	CG ASP OD1 ASP	663 663	59. 668 68. 925 32. 606 1. 00 13. 51 59. 476 67. 692 32. 633 1. 00 14. 06	A C	
ATOM	5134	OD2 ASP	663	58. 809 69. 758 32. 962 1. 00 11. 87	A 0 A 0	
ATOM	5135	C ASP	663	60. 807 71. 625 33. 300 1. 00 13. 03	A C	
ATOM	5136	0 ASP	663	60.036 71.713 34.260 1.00 12.71	A O	
ATOM ATOM	5137	N SER	664	60. 945 72. 576 32. 383 1. 00 12. 83	A N	
ATOM	5138 5139	CA SER CB SER	664 664	60. 210 73. 829 32. 425 1. 00 13. 80	A C	
ATOM		OG SER	664	60. 433 74. 600 31. 120 1. 00 14. 92 59. 996 73. 851 30. 000 1. 00 14. 78	A C	
ATOM	5141	C SER	664	58. 715 73. 688 32. 674 1. 00 13. 35	A O	
ATOM		0 SER	664	58. 234 73. 974 33. 762 1. 00 15. 82	A O	
ATOM		N VAL	665	57. 987 73. 247 31. 658 1. 00 13. 43	A N	
ATOM	5144	CA VAL	665	56. 540 73. 101 31. 733 1. 00 14. 34	A C	

					FIC	G. 4-	106			(Continued)
					1, 1,	J. 4	100	•		
ATOM	5145	CB	VAL	665	56.027	72. 182	30.602	1.00 14.98	Α	С
ATOM	5146	CG1		665	54. 496	72.131	30.615	1.00 15.10	Ä	Č
ATOM	5147		VAL	665	56. 537	72.690	29. 263	1.00 13.19	Ä	č
ATOM	5148	C	VAL	665	55. 972	72.620	33.070	1.00 14.50	A	č
ATOM	5149	ŏ	VAL	665	55. 153	73. 302	33.677	1.00 14.33	A	ŏ
ATOM	5150	Ň	TYR	666	56. 392	71.452	33. 534	1.00 15.45	A	Ň
ATOM	5151	CA	TYR	666	55. 876	70. 948	34. 801	1.00 17.06	A	Č
ATOM	5152	CB	TYR	666	56. 323	69. 501	35. 038	1.00 15.58	A	Č
ATOM	5153	CG	TYR	666	55. 839	68. 903		1.00 13.94	Ä	
ATOM	5154		TYR	666	54. 692	68. 119	36. 395	1.00 13.34	A	C C
ATOM	5155		TYR	666	54. 276	67. 517	37. 577	1.00 14.70	A	C
ATOM	5156		TYR	666	56. 560	69. 080	37. 534	1.00 13.28		C
ATOM	5157		TYR	666	56. 154	68. 482	38. 727	1.00 13.77	A	C
ATOM	5158	CZ	TYR	666	55. 012	67. 700	38. 737	1.00 12.27	A	C
ATOM	5159	OH	TYR	666	54. 609	67. 072	39. 896	1.00 13.32	A	C
ATOM	5160	C	TYR	666	56. 297	71. 796	35. 998	1.00 13.37	A	0
ATOM	5161	Õ	TYR	666	55. 451	72. 200	36. 795	1.00 17.89	A	C
ATOM	5162	N	THR	667	57. 592	72. 266	36. 125	1.00 19.29	A	O N
ATOM	5163	CA	THR	667	58. 092	72.833	37. 265	1.00 17.90	A	
ATOM	5164	CB	THR	667	59. 621	72. 953	37. 251	1.00 19.74	Α Α	C
ATOM	5165	0G1		667	60. 206	71.675	36.968	1.00 10.04	A	C
ATOM	5166		THR	667	60. 108	73. 441	38. 604	1.00 20.16	A	0
ATOM	5167	C	THR	667	57. 537	74. 246	37. 339	1.00 17.74	A	C
ATOM	5168	Õ	THR	667	56. 916	74. 635	38. 333	1.00 21.44	A	C
ATOM	5169	N	GLU	668	57. 7.78	75.011	36. 280	1.00 21.31	A	0 N
ATOM	5170	CA	GLU	668	57. 330	76. 389	36. 200	1.00 21.00	A	N C
ATOM	5171	CB	GLU	668	57. 746	76. 976	34. 859	1.00 21.18	A	C
ATOM	5172	CG	GLU	668	59. 251	77. 096	34. 703	1.00 20.09	A	C
ATOM	5173	CD	GLU	668	59. 657	77. 559	33. 322	1.00 20.20	A	C
ATOM	5174		GLU	668	58. 783	78. 068	32. 588	1.00 19.33	A	C
ATOM	5175		GLU	668	60. 851	77. 422	32. 977		A	0
ATOM	5176	C	GLU	668	55. 828	76. 517	36. 394	1.00 18.34 1.00 21.50	A	0
ATOM	5177	Ö	GLU	668	55. 339	77. 559	36. 814	1.00 21.30	A	C
ATOM	5178	N	ARG	669	55. 098	75. 449	36. 101	1.00 22.31	A	0 N
ATOM	5179	CA	ARG	669	53.648	75. 458	36. 249	1.00 21.30	A	N
ATOM	5180	CB	ARG	669	53.060	74. 121	35. 786	1.00 21.16	A	C C
ATOM	5181	CG	ARG	669	51.546	74. 026	35. 922		A	
ATOM	5182	CD	ARG	669	51.085	72. 625		1.00 21.37	A	C
ATOM	5183	NE	ARG	669		72. 187	35. 653	1.00 20.85	A	C
ATOM	5184	CZ	ARG	669	51.467		34. 319	1.00 21.84	A	N C
ATOM	5185		ARG	669	51.667 51.522	70. 918 69. 962	33. 981	1.00 21.10	A	C
ATOM	5186		ARG	669			34. 888	1.00 19.62	A	N
ATOM	5187	C	ARG	669	52. 018	70.610	32.741	1.00 20.23	A	N C
ATOM	5188	Ö	ARG	669	53. 246	75. 706	37.695	1.00 21.23	A	C
ATOM	5189	N	TYR	670	52. 209 54. 067	76. 306 75. 239	37. 957	1.00 20.45	A	0 at
ATOM	5190	CA	TYR	670	53.771	75. 409	38. 631 40. 047	1.00 21.65 1.00 22.27	A	N C
ATOM	5191	CB	TYR	670	53. 752	75. 409	40. 764	1.00 22.27	A	C
ATOM	5192	CG	TYR	670	53. 113	72. 930	39. 972	1.00 21.10	A	C
ATOM	5193		TYR	670	53. 896	71.995	39. 310	1.00 20.47	A	C C
WIOII	0100	י עט	1 1 1/	010	UU. UJU	11. 330	JJ. JIV	1.00 60.14	Α	U

					FI	G. 4-	107			(Conti	inued)
ATOM	5194		TYR	670	53. 321		38. 537	1.00 22.18	A	С	
ATOM	5195		TYR	670	51.726		39.850	1.00 19.78	Α	С	
ATOM	5196		TYR	670	51.139		39.079	1.00 19.87	Α	C	
ATOM	5197	CZ	TYR	670	51.944		38.422	1.00 22.17	Α	С	
ATOM	5198	OH	TYR	670	51.388		37. 623	1.00 23.11	Α	0	
ATOM	5199	C	TYR	670	54.769			1.00 23.32	A	C	
ATOM	5200	0	TYR	670	54.442			1.00 24.86	A	0	
ATOM	5201	N	MET	671	55. 983			1.00 24.66	A	N	
ATOM	5202	CA	MET	671	57. 029		40.851	1.00 23.96	Ą	C	
ATOM	5203	CB	MET	671	58. 327		40. 905	1.00 24.00	A	C	
ATOM	5204	CG	MET	671	58. 288		41.852	1.00 23.55	A	C	
ATOM	5205	SD	MET	671	58. 383		43. 565	1.00 24.97	A	S	
ATOM	5206	CE	MET	671	60.159		43. 721	1.00 21.94	A	C	
ATOM ATOM	5207 5208	C	MET MET	671 671	57. 330		40. 203	1.00 24.00	A	C	
ATOM	5208	O N	GLY	672	58. 101		40. 756	1.00 25.98	A	0	
ATOM	5210	CA	GLY	672	56. 741 57. 044		39. 045	1.00 22.07	A	N	
ATOM	5211	CA	GLY	672	58.472		38. 379 37. 857	1.00 22.40 1.00 22.69	A	C C	
ATOM	5212	ŏ	GLY	672	59. 005		37.641	1.00 22.03	A A	0	
ATOM	5213	N	LEU	673	59. 108		37. 667	1.00 23.21	A	N	
ATOM	5214	CA	LEU	673	60. 477		37. 151	1.00 20.90	A	C	
ATOM	5215	CB	LEU	673	60. 626		36. 164	1.00 19.50	A	Č	
ATOM	5216		LEU	673	59.639		35.010	1.00 19.96	A	č	
ATOM	5217		LEU	673	59. 779		34. 147	1.00 20.87	Ä	č	
ATOM	5218		LEU	673	59. 892		34. 203	1.00 21.63	Ä	č	
ATOM	5219	C	LEU	673	61.528		38. 248	1.00 21.08	A	Č	
ATOM	5220	0	LEU	673	61.313		39. 239	1.00 21.87	A	Ō	
ATOM	5221	N	PRO	674	62.692	80.700	38.072	1.00 21.90	Α	N	
ATOM	5222	CD	PRO	674	63. 050		36.968	1.00 21.16	Α	С	
ATOM	5223	CA	PR0	674	63. 780		39.050	1.00 23.23	Α	С	
ATOM	5224	CB	PRO	674	64.618		38. 709	1.00 21.90	Α	С	
ATOM	5225	CG	PRO	674	63. 803		37. 695	1.00 22.34	A	С	
ATOM	5226	C	PRO	674	64.617		38. 943	1.00 24.90	A	C	
ATOM	5227	0	PRO	674	65. 841	81. 977	39. 028	1.00 26.10	A	0	
ATOM	5228	N	THR	675	63.966		38. 743	1.00 25.88	A	N	
ATOM	5229	CA	THR	675	64. 695	84. 411	38. 640	1.00 27.60	A	C	
ATOM	5230	CB	THR					1.00 27.12	A	C	
ATOM	5231	OG1		675	62. 811	85. 524	37. 599	1.00 29.30	A	0	
ATOM	5232	CG2		675	64. 431	84. 471	36. 156	1.00 25.59	A	C	
ATOM ATOM	5233 5234	C 0	THR THR	675	64. 496	85. 211	39. 918	1.00 28.74	A	C	
ATOM	5235		PRO	675 676	63. 543	84. 982	40.660	1.00 29.47	A	0	
ATOM	5236		PRO	676	65. 404 66. 625	86. 156 86. 508	40. 200	1.00 29.41	A	N	
ATOM	5237		PRO	676	65. 284	86.969	39. 457 41. 411	1.00 28.96 1.00 29.70	A	C	
ATOM	5238		PRO	676	66.465	87. 929	41. 411	1.00 29.70	A A	C C	
ATOM	5239		PRO	676	67. 467	87. 142	40. 533	1.00 28.87	A A	C	
ATOM	5240	C	PRO	676	63. 948	87. 707	41. 484	1.00 20.27	A A	C	
ATOM	5241	Ŏ	PRO	676	63. 359	87. 829	42. 558	1.00 29.93	A	0	
ATOM	5242	Ň	GLU	677	63.463	88. 190	40. 343	1.00 29.33	A	N	
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	14			FI	G. 4-	1 0 8			
ATOM	5243	CA GLI	J 677	62. 203	88. 923	40.348	1.00 30.92	Α	C
ATOM	5244	CB GL	J 677	62.192		39.264	1.00 32.38	A	C
ATOM	5245	CG GEU	J 677	62. 103		37.821	1.00 34.78	A	C
ATOM	5246	CD GLI		63. 380		37. 331	1.00 37.04	A	C
ATOM	5247	OE1 GL		64.480		37.697	1.00 35.11	A	0
ATOM	5248	OE2 GL		63. 276		36.566	1.00 37.80	A	0
ATOM	5249	C GL		60. 952		40. 231	1.00 30.10	A	C
ATOM	5250	0 GL		59. 893		39.849	1.00 31.67	A	0
ATOM	5251	N AS		61.067		40.546	1.00 28.40	A	N C
ATOM	5252	CA AS		59.906		40.523	1.00 26.09 1.00 25.88	A A	C
ATOM	5253	CB AS		59. 833		39. 253 39. 097	1.00 23.00	A	C
ATOM	5254	CG AS		58. 472 57. 885		40.128	1.00 28.22	Ä	ŏ
ATOM	5255	OD1 AS		57. 980		37.956	1.00 28.80	A	ŏ
ATOM ATOM	5256 5257	OD2 AS: C AS:		59. 920		41.737	1.00 25.86	A	č
ATOM	5258	0 AS		59. 481		42.810	1.00 28.55	. A	. 0
ATOM	5259	N AS		60. 442		41.591	1.00 23.97	A	N
ATOM	5260	CA AS		60. 443		42.708	1.00 21.47	A	C
ATOM	5261	CB AS		59. 326		42.496	1.00 19.41	Α	С
ATOM	5262	CG AS		58. 894		43.778	1.00 19.58	Α	С
ATOM	5263	OD1 AS		58. 491		43.775	1.00 20.44	Α	0
ATOM	5264	ND2 AS		58.957		44.882	1.00 18.70	A	N
MOTA	5265	C AS		61.760		42.957	1.00 21.79	A	C
ATOM	5266	0 AS		61.770		43.601	1.00 21.89	A	0
ATOM	5267	N LE		62. 873		42. 472	1.00 24.38	A	И.
ATOM	5268	CA LE		64. 164		42.665	1.00 26.33	A	C
ATOM	5269	CB LE		65. 316		42.157	1.00 26.74	A	C
ATOM	5270	CG LE		66. 726		42.385	1.00 28.22	A	C
ATOM	5271	CD1 LE		66.844		41.747 41.801	1.00 30.03 1.00 29.33	A A	C C
ATOM	5272	CD2 LE		67. 772 64. 449		44. 109	1.00 23.33	Ā	C
ATOM	5273 5274	C LE		64. 977		44. 347	1.00 28.31	Ä	ŏ
ATOM ATOM	5275	N AS		64.111		45. 072	1.00 27.79	A	N
ATOM	5276	CA AS		64. 360		46. 475	1.00 28.03	A	Ĉ
ATOM	5277	CB AS		63. 836		47.394	1.00 30.36	A	Č
ATOM	5278	CG AS		64.774		47.473	1.00 34.23	Α	C
ATOM	5279	OD1 AS					1.00 35.59	Α	0
ATOM	5280	OD2 AS		64.380		48.067	1.00 36.71	Α	0
ATOM	5281	C AS		63. 773		46.920	1.00 27.55	Α	C
ATOM	5282	Q AS	P 681	64. 428		47.647	1.00 28.05	Α	0
ATOM	5283	N HI		62.55 1		46.502	1.00 25.37	Α	N
ATOM	5284	CA HI		61.981		46.913	1.00 25.07	A	C
ATOM	5285	CB HI		60.450		46.801	1.00 25.14	A	C
ATOM	5286	CG HI		59. 833		47. 349	1.00 27.18	A	C
ATOM	5287	CD2 HI		59. 09		46.754	1.00 27.87	A	C
ATOM	5288	ND1 HI		60.021		48.650	1.00 26.29	A	N
ATOM	5289	CE1 HI		59. 428		48.832	1.00 26.61	A	C
ATOM	5290	NE2 HI		58. 85'		47. 697 46. 130	1.00 25.03 1.00 24.30	A A	N C
ATOM	5291	C H	S 682	62. 55	11.300	40.130	1.00 44.00	А	U

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	t								(Continued)
				FIC	3. 4 -	109			
ATOM ATOM ATOM	5292 5293 5294	N 1 CA 1	HIS 682 TYR 683 TYR 683	63. 144 63. 768	76. 837 78. 258 77. 208	46. 572 44. 966 44. 157	1.00 23.47 1.00 23.49 1.00 22.64	A A A	0 N C
ATOM ATOM	5295 5296	CG 7	FYR 683 FYR 683	63. 291	77. 758 77. 594	42. 812 41. 655	1.00 20.68 1.00 19.28	A A	C C
ATOM ATOM	5297 5298	CD1 7 CE1 7			76. 461 76. 317	40.857 39.783	1.00 16.29 1.00 16.83	A A	C C
ATOM ATOM	5299 5300	CD2 7 CE2 7	TYR 683	62.361	78. 589 78. 453	41.347 40.276	1.00 20.47 1.00 20.17	Α	C
ATOM	5301	CZ 1	FYR 683	61.554	77. 314	39.500	1.00 19.09	A A	C C
ATOM ATOM	5302 5303		FYR 683 FYR 683		77. 176 76. 727	38. 441 44. 924	1.00 21.54 1.00 22.32	A A	0 C
ATOM ATOM	5304 5305	0 1	ΓYR 683 ARG 684	65.189	75. 533	45. 125	1.00 22.65	A	0
ATOM	5306	CA A	ARG 684	67.025	77. 685 77. 392	45. 355 46. 076	1.00 22.44 1.00 22.97	A A	N C
ATOM ATOM	5307 5308		ARG 684 ARG 684		78. 624 79. 064	46. 071 44. 672	1.00 22.89 1.00 24.57	A A	C C
ATOM ATOM	5309 5310	CD A	ARG 684 ARG 684	69. 238	78. 020 78. 223	44. 004 42. 562	1.00 23.11 1.00 25.47	Α	C
ATOM	5311	CZ A	ARG 684	69. 844	79. 299	41.974	1.00 27.89	A A	N C
ATOM ATOM	5312 5313	NH1 A NH2 A	\RG 684 \RG 684		80. 294 79. 388	42. 703 40. 648	1.00 29.09 1.00 27.04	A A	N N
ATOM ATOM	5314 5315		\RG 684 \RG 684	66. 807	76. 922 76. 368	47. 501 48. 111	1.00 22.90 1.00 24.16	Α	C
ATOM	5316	N A	ASN 685	65.608	77.121	48.030	1.00 24.64	A A	O N
ATOM ATOM	5317 5318		ASN 685 ASN 685	65. 331 64. 599	76. 715 77. 831	49. 399 50. 134	1.00 24.41 1.00 28.42	A A	C C
ATOM ATOM	5319 5320		ASN 685	64.455	77.547	51.610	1.00 34.24	· A	C
ATOM	5321	ND2 A	ISN 685	65. 410 63. 264	77. 117 77. 791	52. 266 52. 150	1.00 38.25 1.00 37.49	. A A	O N
ATOM ATOM	5322 5323		ISN 685 ISN 685	64. 545 64. 356	75. 419 74. 929	49. 537 50. 649	1.00 23.72 1.00 23.86	A A	C 0
ATOM ATOM	5324 5325	N S	SER 686 SER 686	64. 101 63. 336	74. 852 73. 613	48.417	1.00 21.55	Α	N
ATOM	5326	CB S	SER 686	61.976	73.811	48. 457 47. 774	1.00 19.71 1.00 19.20	A A	C C
ATOM ATOM	5327 5328		SER 686 SER 686	62.114 64.060	74. 112 72. 421	46. 397 47. 823	1.00 15.00 1.00 20.13	A A	0 C
ATOM ATOM	5329 5330	0 S	SER 686 HR 687	63.447	71.611	47.128	1.00 21.27	A	0
ATOM	5331	CA T	HR 687	65. 362 66. 122	72. 307 71. 189	48. 060 47. 509	1.00 19.02 1.00 17.15	A A	N C
ATOM ATOM	5332 5333	CB T OG1 T	HR 687 HR 687	67. 441 68. 362	71.665 71.959	46. 906 47. 960	1. 00 16. 10 1. 00 17. 42	A A	C 0
ATOM ATOM	5334 5335	CG2 T	HR 687	67. 214	72.920	46.058	1.00 14.71	Α	С
ATOM	5336	0 T	HR 687	66. 433 66. 496	70. 153 70. 466	48. 585 49. 763	1. 00 15. 79 1. 00 15. 82	A A	C 0
ATOM ATOM	5337 5338		AL 688 AL 688	66. 627 66. 935	68. 908 67. 854	48. 182 49. 147	1. 00 18. 43 1. 00 17. 92	A A	N C
ATOM ATOM	5339 5340		'AL 688	66.840	66.453	48.480	1.00 17.13	A	C
WIOI	0040	COI Y	UL 000	67.092	65. 352	49.503	1.00 15.01	· А	С

										(Continued)
••					FIC	G. 4-	1 1 0			,
ATOM	5341	CG2	VAI.	688	65. 459	66. 279	47. 845	1.00 18.49	A	С
ATOM	5342		VAL	688	68. 341	68.059	49.720	1.00 17.50	Α	C
ATOM	5343		VAL	688	68. 559		50.923	1.00 15.69	Α	0
ATOM	5344		MET	689	69. 280		48.851	1.00 16.92	Α	N
ATOM	5345		MET	689	70.672	68.647	49. 246	1.00 17.40	A	C
ATOM	5346		MET	689	71.475		48.065	1.00 13.91	A	C
ATOM	5347	CG	MET	689	71.829		46. 984	1.00 10.55	A	C
ATOM	5348		MET	689	70.465		45. 909	1.00 11.73	A	S
ATOM	5349		MET	689	70. 338		44.871	1.00 9.36	A	C
ATOM	5350	C	MET	689	70. 897	69. 539	50.479	1.00 17.90	A	C
ATOM	5351	0	MET	689	71. 721	69. 220	51.341	1.00 16.90	A	0 N
ATOM	5352	N	SER	690	70.179		50.569	1.00 18.32	A	N
ATOM	5353	CA	SER	690	70. 358		51.712	1.00 21.65	A	C
ATOM	5354	CB	SER	690	69. 621	72. 866	51.501 51.711	1.00 20.29 1.00 24.78	A	C 0
ATOM	5355	OG C	SER	690	68. 234		53. 038	1.00 24.18	A A	C
ATOM	5356	C	SER	690	69. 898 69. 930		54.063	1.00 22.31	A	0
ATOM	5357 5358	O N	SER ARG	690 691	69. 480		53.023	1.00 21.70	A	N
ATOM ATOM	5359	CA	ARG	691	69. 041		54. 249	1.00 23.07	Ä	Ċ
ATOM	5360	CB	ARG	691	67. 591		54.113	1.00 22.90	A	Č
ATOM	5361	CG	ARG	691	66. 623		53. 770	1.00 22.81	Ä	č
ATOM	5362	CD	ARG	691	65. 201		53. 813	1.00 22.97	Ä	Č
ATOM	5363	NE	ARG	691	64. 236		53.694	1.00 24.03	A	N
ATOM	5364	CZ	ARG	691	62.963		54.061	1.00 26.18	Α	С
ATOM	5365	NH1		691	62.509		54.566	1.00 25.20	Α	N
ATOM	5366	NH2		691	62.149		53.946	1.00 26.01	Α	N
ATOM	5367	С	ARG	691	69.922		54. 593	1.00 24.24	Α	С
ATOM	5368	0	ARG	.691	69. 595		55.488	1.00 25.28	A	0
ATOM	5369	N	ALA	692	71.041		53.889	1.00 24.03	A	N
ATOM	5370	CA	ALA	692	71.960		54. 100	1.00 24.84	A	C
ATOM	5371	CB	ALA	692	73. 270		53.360	1.00 24.20	A	C
ATOM	5372	C	ALA	692	72. 251		55. 562	1.00 24.60	A	C
ATOM	5373	0	ALA	692	72.066		55.967	1.00 24.83	A	0 N
ATOM	5374	N	GLU	693	72. 707		56.347	1.00 25.74 1.00 27.13	A	N C
ATOM	5375	CA	GLU	693	73.033		57. 757 58. 463	1.00 27.13	A A	Č
ATOM	5376	CB	GLU GLU	693	73. 351 74. 829		58. 583	1.00 25.38	A	C
ATOM ATOM	5377 5378	CG CD	GLU	693 693	75.604		59. 463	1.00 39.02	A	Č
ATOM	5379		GLU	693	74. 984		60.316	1.00 38.42	A	ő
ATOM	5380		GLU	693	76. 845		59. 307	1.00 41.03	Ä	Ŏ
ATOM	5381	C	GLU	693	71.947		58. 549	1.00 26.16	Ä	Č
ATOM	5382	ŏ	GLU	693	72. 250		59. 506	1.00 26.78	Ä	ő
ATOM	5383	Ň	ASN	694	70. 688		58.160	1.00 24.46	Ä	Ň
ATOM	5384	CA	ASN	694	69. 594		58.873	1.00 24.35	A	Ċ
ATOM	5385	CB	ASN	694	68. 274		58.619	1.00 26.79	A	Č
ATOM	5386	ĊĠ	ASN	694	68. 191		59.370	1.00 28.23	Α	С
ATOM	5387		ASN	694	67. 291		59.132	1.00 29.60	Α	0
ATOM	5388	ND2	ASN	694	69. 127	68.015	60. 287	1.00 27.09	A	N
ATOM	5389	C	ASN	694	69.412	64. 252	58. 567	1.00 22.78	Α	C

ATOM

5438

CB

TYR

700

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(Continued) FIG. 4 - 111 0 68.736 59.318 1.00 22.09 63.555 Α **ATOM** 5390 0 ASN 694 70.008 N 63.764 57.481 1.00 21.23 A ATOM 5391 N PHE 695 C 69.876 62.351 57.135 1.00 20.87 Α **ATOM** 5392 CA PHE 695 C 62.085 55.686 1.00 18.97 70.297 A **ATOM** 5393 CB PHE 695 1.00 15.41 C 54.663 69.262 62.465 A **ATOM** 5394 CG PHE 695 C 68.980 54.394 ATOM 5395 CD1 PHE 695 63.804 1.00 16.20 A Ċ 68.582 53.948 5396 CD2 PHE 695 61.480 1.00 13.85 A ATOM C 68.033 64.160 53.419 PHE 695 1.00 15.80 A **ATOM** 5397 CE1 67.636 C 61.819 52.976 1.00 14.69 A CE2 PHE 695 **ATOM** 5398 67.360 63.165 52.710 1.00 14.36 A 5399 CZPHE 695 **ATOM** C 70.704 61.478 58.068 1.00 22.60 Α C PHE 695 ATOM 5400 57.932 0 70.734 60.253 1.00 22.75 Α PHE **ATOM** 5401 0 695 71.388 N LYS 696 62.111 59.014 1.00 23.86 A **ATOM** 5402 N 72.189 61.369 59.980 C LYS 696 1.00 24:30 A ATOM 5403 CA 73.119 C LYS 62.315 60.744 1.00 23.88 5404 CB A ATOM 696 LYS 74. 230 62.883 59.891 1.00 27.19 C CG A ATOM 5405 696 63. 793 60.672 C 75.160 1.00 26.74 CD LYS 696 A ATOM 5406 Ċ 76.354 64.211 59.816 1.00 26.44 ATOM CE LYS 696 A 5407 77.248 LYS 65.163 60.534 1.00 28.88 N ATOM NZ A 5408 696 71. 256 60.670 60.962 1.00 24.58 C 5409 696 ATOM C LYS A 61.710 ATOM LYS 696 71.673 59.790 1.00 24.47 0 5410 0 Α 69.986 60.949 ATOM N GLN 697 61.060 1.00 24.66 N 5411 A 69.013 60.476 61.865 1.00 26.18 GLN C ATOM 5412 CA 697 A 62. 385 62. 792 68.072 1.00 28.53 C 61.571 ATOM 5413 CB GLN 697 Α C 697 68.766 62.865 1.00 31.73 **ATOM** 5414 CG GLN A 67.790 GLN 63.938 63.262 1.00 34.90 C ATOM 5415 CD 697 A 63.195 68.086 65.133 0 **ATOM** 5416 0E1 GLN 697 1.00 37.16 A ATOM 5417 NE2 GLN 697 66.627 63.516 63.753 1.00 36.42 N A ATOM 5418 C GLN 697 68.176 59.346 61.259 1.00 24.79 C A 67. 294 68. 439 ATOM 5419 0 GLN 697 58.808 61.9231.00 27.00 0 A 58.979 60.011 VAL 1.00 21.46 N ATOM 5420 N 698 A ATOM 698 67.659 57.922 59.383 1.00 18.56 C 5421 CA VAL A 58.517 5422 CB 698 66.510 58.524 1.00 19.77 C ATOM VAL A 59.467 59.355 698 65.674 C ATOM 5423 CG1 VAL 1.00 19.11 A 57.296 C 698 67.077 59.233 1.00 15.74 ATOM 5424 CG2 VAL A 698 68.469 56.987 58.484 1.00 18.57 **ATOM** 5425 C VAL A C 69.614 5426 0 57.265 58.135 1.00 17.50 **ATOM** VAL 698 A 0 67.850 ATOM 5427 N **GLU** 699 55.868 58.121 1.00 18.32 A. N ATOM 5428 CA **GLU** 699 68.456 54.885 57.236 1.00 18.24 A C ATOM 5429 CB GLU 699 68.007 53.488 57.636 1.00 19.38 A C ATOM 5430 CG **GLU** 699 67.600 53.411 59.097 1.00 26.18 A C ATOM 5431 CD **GLU** 699 68.384 52.377 59.891 1.00 29.91 A **ATOM** 5432 0E1 GLU 699 69.620 52.305 59.712 1.00 31.51 0 A 67.765 67.857 ATOM 5433 0E2 GLU 699 51.651 60.703 1.00 30.28 A 0 55.891 ATOM 5434 C **GLU** 699 55.286 1.00 17.20 A C ATOM 5435 0 **GLU** 699 66.638 55.397 55.765 1.00 16.35 A 0 ATOM 5436 N **TYR** 700 68.714 55.516 54.899 1.00 15.53 N A **ATOM** 5437 700 68.275 55.968 53.584 1.00 12.51 C CA TYR A

57.383 **SUBSTITUTE SHEET (RULE 26)**

53. 365

1.00 12.28

68.810

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										(Continued)
					FIG	. 4 -	112			(Oontinueu)
				700	00.074	FO 10F	FO 114	1 00 12 02	A	C
ATOM	5439	CG	TYR	700	68. 374	58. 105	52. 114 51. 746	1.00 13.03 1.00 12.78	A	C C
ATOM	5440	CD1		700	67.027	58. 171 58. 961	50.666	1.00 12.78	A A	C
ATOM	5441	CE1		700	66.611	58. 840	51. 359	1.00 1.34	A	C
MOTA	5442	CD2		700	69. 301 68. 895	59. 629	50. 282	1.00 12.31	A	Č
ATOM	5443		TYR	700		59.688	49. 948	1.00 10.45	A	Č
ATOM	5444	CZ	TYR	700	67. 550 67. 150	60. 495	48. 913	1.00 10.00	A	ŏ
ATOM	5445	OH C	TYR	700 700	68.743	55. 056	52.468	1.00 0.31	A	Č
ATOM	5446	C	TYR TYR	700	69. 881	54. 594	52.463	1.00 10.84	Ä	ŏ
ATOM	5447	O N	LEU	701	67. 836	54. 775	51.540	1.00 10.04	A	N
MOTA	5448	CA	LEU	701	68. 142	53. 950	50. 383	1.00 11.02	A	Ċ
ATOM	5449 5450	CB	LEU	701	67. 313	52.667	50. 378	1.00 8.96	A	č
ATOM ATOM	5450 5451	CG	LEU	701	67.439	51.794	49. 123	1.00 10.04	Ä	č
ATOM	5452	CD1		701	68. 841	51.873	48. 511	1.00 7.25	Ä	č
ATOM	5453	CD2		701	67. 089	50.376	49.490	1.00 5.44	A	č
ATOM	5454	CDZ	LEU	701	67.811	54. 799	49. 170	1.00 13.03	Ä	Č
ATOM	5455	ŏ	LEU	701	66.660	55. 219	48. 986	1.00 13.35	A	Ö
ATOM	5456	N	LEU	702	68. 840	55.068	48. 367	1.00 12.91	Ä	Ň
ATOM	5457	ĊA	LEU	702	68. 724	55. 888	47.169	1.00 11.74	A	C
ATOM	5458	CB	LEU	702	69. 806	56.968	47. 196	1.00 11.17	A	C
ATOM	5459	CG	LEU	702	69.916	57.965	46.044	1.00 12.13	Α	C
ATOM	5460		LEU	702	68. 569	58.656	45.803	1.00 10.71	Α	C
ATOM	5461		LEU	702	71.006	58.981	46.368	1.00 10.37	Α	C
ATOM	5462	C	LEU	702	68.883	55.003	45.942	1.00 13.49	Α	С
ATOM	5463	0	LEU	702	69.854	54.251	45.832	1.00 14.04	Α	0
ATOM	5464	N	ILE	703	67. 935	55.111	45.016	1.00 13.82	Α	N
ATOM	5465	CA	ILE	703	67. 934	54. 297	43.806	1.00 12.92	Α	С
ATOM	5466	CB	ILE	703	66.931	53. 152	43.964	1.00 12.98	Α	С
ATOM	5467		ILE	703	66. 897	52.305	42.706	1.00 15.12	A	C
ATOM	5468	CG1	ILE	703	67. 299	52. 322	45. 196	1.00 13.52	Α	C
ATOM	5469	CD1	ILE	703	66. 202	51.383	45.663	1.00 13.28	Α	C
ATOM	5470	C	ILE	703	67. 561	55. 125	42. 582	1.00 14.12	Α	C
ATOM	5471	0	ILE	703	66. 635	55. 938	42.629	1.00 15.85	Α	0
ATOM	5472	N	HIS	704	68. 265	54. 909	41.473	1.00 13.28	A	N
ATOM	5473	CA	HIS	704	67. 987	55.678	40. 265	1.00 11.81	Ą	C
ATOM	5474	CB	HIS	704	68.670	57.048	40. 391	1.00 11.13	A	C
ATOM	5475	CG	HIS	704	67.968	58. 156	39.667	1.00 11.66	A	C
ATOM	5476		HIS	704	67. 446	58. 221	38. 418	1.00 10.83	A	C
ATOM	5477		HIS	704	67. 736	59.387	40. 244	1.00 10.07	A	N
ATOM	5478		HIS	704	67. 098	60.162	39. 385	1.00 9.04	A	Ç
ATOM	5479		HIS	704	66.910	59.479	38. 270	1.00 11.23	A	N
ATOM	5480	C	HIS	704	68. 464	54.965	38. 992	1.00 11.87	A	C
ATOM	5481	0	HIS	704	69. 503	54.306	38. 980	1.00 11.87	A	0
ATOM	5482	N	GLY	705	67. 684	55.082	37. 926	1.00 11.49	A	N
ATOM	5483	CA	GLY	705	68.075	54. 486	36.663	1.00 11.90	A	C
ATOM	5484	C	GLY	705	69.066	55. 449	36. 036	1.00 12.16	A	C 0
ATOM	5485 5486	0 N	GLY	705 706	68.911	56.660	36. 153 35. 372	1. 00 13. 94 1. 00 13. 29	A A	N N
ATOM ATOM	5486 5487	N CA	THR THR	706	70. 086 71. 101	54. 928 55. 782	35. 312	1.00 13.29	A	C
VION	0401	υA	1111/	100	(1.101	JJ. 104	34. 110		n	U

					(Continued)
				FIG. 4-113	(
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	5488 5489 5491 5492 5493 5494 5495 5496 5497 5498 5499 5500 5501 5502 5503 5504 5509 5511 5512 5513 5514 5515 5516 5517 5518 5519 5520 5521 5522 5523 5524 5525	OG1 THR CG2 THR C THR N ALA CA ALA CB ALA C ALA O ALA N ASP CA ASP CB ASP CB ASP OD1 ASP OD2 ASP C ASP OD1 ASP CA ASP CB ASP CB ASP CC ASP OD1 ASP CA ASP CB ASP CC ASP OD1 ASP CC ASP OD2 ASP CC ASP OD1 ASP CC ASP OD2 ASP CC ASP OD3 ASP CC ASP OD4 ASP CC ASP OD5 ASP CC ASP OD6 ASP N ASN CC	706 706 706 706 706 707 707 707 707 707	72. 417 55. 001 34. 557 1. 00 11. 94 A 72. 230 53. 983 33. 565 1. 00 12. 79 A 72. 840 54. 344 35. 861 1. 00 12. 66 A 70. 678 56. 409 33. 455 1. 00 13. 02 A 71. 183 57. 461 33. 084 1. 00 14. 35 A 69. 754 55. 770 32. 748 1. 00 13. 82 A 69. 289 56. 302 31. 469 1. 00 15. 26 A 69. 126 55. 176 30. 442 1. 00 13. 60 A 67. 970 57. 030 31. 644 1. 00 16. 56 A 67. 154 57. 075 30. 720 1. 00 17. 71 A 67. 154 57. 600 32. 828 1. 00 16. 56 A 67. 154 57. 600 32. 828 1. 00 16. 71 A 66. 534 58. 314 33. 113 1. 00 16. 71 A 64. 957 58. 834 35. 000 1. 00 19. 59 A 64. 498 58. 317 36. 038 1. 00 19. 59 A 65. 715 <	0 N C C C O O C C O N C C C O N C O N C C C O N C C C O N C C C O N C C C O N C C C O N C C C O N C C C C
					C C C
ATOM ATOM	5527 5528	C VAL O VAL	711 711	65. 645 62. 237 36. 038 1. 00 10. 48 A 65. 949 61. 068 36. 280 1. 00 10. 00 A	C O
ATOM ATOM	5529 5530	N HIS	712 712	66. 518 63. 126 35. 591 1. 00 10. 94 A 67. 899 62. 758 35. 302 1. 00 11. 74 A	N C
ATOM ATOM ATOM	5531 5532 5533	CB HIS CG HIS CD2 HIS	712 712 712	68. 577 63. 961 34. 646 1. 00 10. 79 A 67. 782 64. 529 33. 514 1. 00 11. 58 A 66. 855 63. 955 32. 705 1. 00 12. 39 A	C
ATOM ATOM	5534 5535	ND1 HIS CE1 HIS	712 712 712	66. 855 63. 955 32. 705 1. 00 12. 39 A 67. 833 65. 858 33. 154 1. 00 11. 87 A 66. 966 66. 082 32. 181 1. 00 12. 19 A	C N C
ATOM	5536	NE2 HIS	712	66. 359 64. 944 31. 891 1. 00 11. 62 A SUBSTITUTE SHEET (RULE 26)	Ň

					(Continued)
				FIG. 4-114	(Continued)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	5537 5538 5539 5540 5541 5543 5544 5545 5555 5556 5556 5556 5566 556	C HIS O HIS N PHE CA PHE CG PHE CG PHE CCD1 PHE CCD2 PHE CCD2 PHE CCD2 PHE CCD PHE CCD CD GLN CCD GLN	712 713 713 713 713 713 713 713 713 713 714 714 714 714 714 714 715 715 715 715 715 715	68. 698 62. 222 36. 491 1. 00 10. 63 68. 461 62. 598 37. 633 1. 00 11. 98 69. 631 61. 319 36. 210 1. 00 10. 82 70. 458 60. 720 37. 251 1. 00 11. 00 71. 533 59. 823 36. 634 1. 00 11. 14 72. 270 58. 989 37. 639 1. 00 11. 47 71. 714 57. 813 38. 126 1. 00 11. 22 73. 496 59. 407 38. 144 1. 00 11. 84 72. 367 57. 066 39. 109 1. 00 11. 98 74. 153 58. 667 39. 126 1. 00 13. 82 73. 586 57. 495 39. 610 1. 00 11. 04 71. 122 61. 818 38. 061 1. 00 11. 85 71. 404 61. 640 39. 243 1. 00 13. 14 71. 377 62. 948 37. 403 1. 00 12. 47 72. 001 64. 113 38. 022 1. 00 10. 55 71. 851 65. 321 37. 082 1. 00 10. 55 71. 851 65. 321 37. 082 1. 00 10. 55 71. 851 65. 321 37. 082 1. 00 10. 55 71. 501 67. 827 36. 891 1. 00 9. 77 70. 447 67. 693 36. 268 1. 00 10. 50 72. 201 68. 948 36. 870 1. 00 9. 43 71. 355 64. 417 39. 368 1. 00 9. 91 72. 037 64. 700 40. 356 1. 00 8. 86 70. 029 64. 340 39. 395 1. 00 10. 27 69. 255 64. 616 40. 599 1. 00 10. 62 67. 771 64. 393 40. 315 1. 00 10. 98 67. 267 65. 219 39. 144 1. 00 11. 10 66. 285 66. 288 39. 567 1. 00 14. 59 66. 381 66. 828 40. 671 1. 00 16. 72 65. 336 66. 613 38. 685 1. 00 12. 90 69. 716 63. 781 41. 780 1. 00 10. 65	(Continued) A
ATOM	5565	NE2 GLN	715	65. 336 66. 613 38. 685 1. 00 12. 90 69. 716 63. 781 41. 780 1. 00 10. 65 69. 976 64. 322 42. 853 1. 00 12. 32 69. 828 62. 472 41. 600 1. 00 9. 91	A N
ATOM ATOM ATOM ATOM ATOM ATOM	5570 5571 5572 5573 5574 5575	CB SER OG SER C SER O SER N ALA CA ALA	716 716 716 716 717 717	69. 937 60. 163 42. 461 1. 00 10. 77 68. 541 59. 994 42. 492 1. 00 14. 60 71. 818 61. 761 42. 876 1. 00 13. 46 72. 341 61. 556 43. 976 1. 00 14. 90 72. 522 62. 094 41. 797 1. 00 12. 22	A C A O A C A O A N
ATOM ATOM ATOM ATOM ATOM ATOM ATOM	5576 5577 5578 5579 5580 5581 5582	CB ALA C ALA O ALA N GLN CA GLN CB GLN CG GLN	717 717 717 717 718 718 718 718	74. 555 62. 487 40. 479 1. 00 12. 46 46 74. 299 63. 423 42. 790 1. 00 13. 73 47 75. 257 63. 375 43. 560 1. 00 15. 24 47 73. 504 64. 482 42. 710 1. 00 13. 27 47 73. 738 65. 631 43. 565 1. 00 13. 07 47 72. 976 66. 841 43. 035 1. 00 13. 93 48	A C A C A C A O A N A C A C
ATOM ATOM	5583 5584 5585	CD GLN OE1 GLN NE2 GLN	718 718 718	74. 996 67. 865 41. 867 1. 00 13. 84 75. 467 68. 172 42. 950 1. 00 16. 85	A C A O A N

			FIG. 4-115	(Continued)
5586 5587 5588 5589 5591 5592 5593 5594 5595 5600 5600 5600 5600 5600 5600 5600	C GLN O GLN N ILE CA ILE CB ILE CG1 ILE CG1 ILE C ILE O ILE N SER CA SER OG SER C SER N LYS CA LYS CA LYS CA LYS CB LYS CC LYS CC LYS NZ LYS C LYS C LYS NZ LYS C	718 718 719 719 719 719 719 719 719 720 720 720 720 721 721 721 721 721 721 721 721 722 722	73. 350 65. 343 45. 026 1. 00 13. 24 73. 941 65. 910 45. 949 1. 00 11. 74 72. 370 64. 460 45. 237 1. 00 12. 01 71. 956 64. 110 46. 594 1. 00 11. 94 70. 691 63. 201 46. 616 1. 00 12. 50 70. 464 62. 673 48. 021 1. 00 11. 09 69. 447 63. 979 46. 174 1. 00 14. 37 68. 170 63. 143 46. 154 1. 00 8. 64 73. 081 63. 338 47. 282 1. 00 11. 72 73. 543 63. 703 48. 367 1. 00 10. 69 73. 508 62. 262 46. 632 1. 00 11. 02 74. 901 60. 325 46. 135 1. 00 11. 02 74. 901 60. 325 46. 135 1. 00 12. 63 75. 471 60. 894 44. 970 1. 00 13. 75 75. 804 62. 207 47. 488 1. 00 12. 18 76. 429 61. 995 48. 537 1. 00 11. 28 76. 159 63. 129 46. 594 1. 00 12. 18 77. 613 64. 82	A C A O N A C C C A C C C C C C C C C C C C C C C C C C C C
5618 5619 5620 5621 5622	CB LEU CG LEU CD1 LEU CD2 LEU C LEU	723 723 723 723 723	74. 626 61. 984 51. 570 1. 00 16. 86 73. 116 62. 205 51. 463 1. 00 18. 78 72. 428 60. 932 50. 991 1. 00 18. 74 72. 576 62. 663 52. 817 1. 00 16. 86 76. 889 62. 926 52. 134 1. 00 17. 26	A C A C A C A C A C A C
5624 5625 5626 5627 5628 5629 5630 5631 5632 5633	N VAL CA VAL CB VAL CG1 VAL CG2 VAL C VAL O VAL N ASP CA ASP CB ASP	724 724 724 724 724 724 724 725 725	77. 641 62. 559 51. 103 1. 00 17. 41 79. 050 62. 234 51. 257 1. 00 16. 64 79. 671 61. 824 49. 902 1. 00 14. 31 81. 187 61. 819 49. 987 1. 00 13. 56 79. 178 60. 449 49. 519 1. 00 14. 78 79. 785 63. 455 51. 803 1. 00 18. 83 80. 665 63. 337 52. 662 1. 00 19. 09 79. 411 64. 632 51. 318 1. 00 19. 19 80. 051 65. 848 51. 776 1. 00 20. 26 79. 627 67. 032 50. 919 1. 00 22. 40	A O A N A C A C A C A C A C A C A C A C A C A O A N A C A C A C
	5587 5588 5589 55991 55993 55995 55995 55995 55996 56001 56005 56006 56006 56007 5611 5612 5622 5622 5622 5622 5622 5632 5632 563	5587 O GLN 5588 N ILE 5589 CA ILE 5591 CG2 ILE 5592 CG1 ILE 5593 CD1 ILE 5594 C ILE 5595 O ILE 5596 N SER 5597 CA SER 5699 OG SER 5600 C SER 5601 O SER 5602 N LYS 5603 CA LYS 5604 CB LYS 5605 CG LYS 5606 CD LYS 5607 CE LYS 5608 NZ LYS 5609 C LYS 5611 N ALA 5612 CA ALA 5613 CB LEU 5620 CD1 LEU	5587 O GLN 718 5588 N ILE 719 5589 CA ILE 719 5590 CB ILE 719 5591 CG2 ILE 719 5592 CG1 ILE 719 5593 CD1 ILE 719 5594 C ILE 719 5595 O ILE 719 5596 N SER 720 5597 CA SER 720 5598 CB SER 720 5599 OG SER 720 5600 C SER 720 5600 C SER 720 5601 O SER 720 5602 N LYS 721 5603 CA LYS 721 5604 CB LYS 721 5605 CG LYS 721 5606 CD LYS 721 5606 CD LYS 721 5607 CE LYS 721 5608 NZ LYS 721 5608 NZ LYS 721 5609 C LYS 721 5610 O LYS 721 5611 N ALA 722 5612 CA ALA 722 5613 CB ALA 722 5614 C ALA 722 5615 O ALA 722 5616 N LEU 723 5617 CA LEU 723 5618 CB LEU 723 5619 CG LEU 723 5610 CD LYS 721 5610 CA LA 722 5611 CD LEU 723 5612 CA LEU 723 5613 CB ALA 722 5614 C ALA 722 5615 O ALA 722 5615 O ALA 722 5616 N LEU 723 5620 CD1 LEU 723 5621 CD2 LEU 723 5622 C LEU 723 5623 O LEU 723 5624 N VAL 724 5625 CA VAL 724 5626 CB VAL 724 5627 CG1 VAL 724 5629 C VAL 724 5630 O VAL 724 5631 N ASP 725 5632 CA ASP 725 5633 CB ASP 725	5586 C GLN 718 73.350 65.343 45.026 1.00 13.24 5587 O GLN 718 73.941 65.910 45.949 1.00 11.74 5588 N ILE 719 72.370 64.460 45.237 1.00 12.01 5589 CA ILE 719 70.691 63.201 46.564 1.00 11.94 5590 CB ILE 719 70.691 63.201 46.594 1.00 11.94 5590 CB ILE 719 70.646 62.673 48.021 1.00 11.09 5592 CG1 ILE 719 68.170 63.143 46.154 1.00 11.72 5593 CD1 ILE 719 73.543 63.333 47.282 1.00 11.32 5594 C ILE 719 73.543 63.733 48.367 1.00 11.32 5595 O ILE 719 73.543 63.733 48.367 1.00 11.32

				n.c. 4 116	(Continued)
				FIG. 4-116	
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	5635 5636 5637 5638 5640 5641 5642 5644 5645 5646 5647 5648 5649	OD1 ASP OD2 ASP C ASP O ASP N VAL CA VAL CB VAL CG1 VAL CG2 VAL C VAL O VAL N GLY CA GLY C GLY O GLY N VAL	725 725 725 726 726 726 726 726 726 727 727 727 727	81. 149 66. 151 49. 319 1. 00 26. 28 A 79. 867 67. 839 48. 704 1. 00 30. 70 A 79. 805 66. 171 53. 238 1. 00 19. 86 A 80. 486 67. 024 53. 792 1. 00 23. 33 A 78. 841 65. 516 53. 873 1. 00 17. 95 A 78. 603 65. 790 55. 285 1. 00 17. 97 A 77. 178 66. 341 55. 567 1. 00 18. 54 A 76. 992 67. 680 54. 875 1. 00 16. 64 A 76. 121 65. 339 55. 120 1. 00 18. 24 A 78. 812 64. 549 56. 124 1. 00 17. 82 A 78. 412 64. 504 57. 283 1. 00 19. 86 A 79. 439 63. 541 55. 535 1. 00 17. 13 A 79. 711 62. 317 56. 263 1. 00 16. 84 A 78. 483 60. 961 57. 794 1. 00 1	0 0 C 0 N C C C C C O N C C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	5651 5652 5653 5654 5655 5656 5657 5658 5669 5660 5661 5662 5663	CA VAL CB VAL CG1 VAL CG2 VAL C VAL O VAL N ASP CA ASP CB ASP CG ASP OD1 ASP OD2 ASP C ASP	728 728 728 728 728 728 729 729 729 729 729 729	76. 331 60. 571 56. 085 1. 00 17. 26 A 75. 030 61. 302 55. 643 1. 00 18. 46 A 73. 838 60. 338 55. 668 1. 00 16. 22 A 74. 753 62. 476 56. 579 1. 00 18. 70 A 76. 411 59. 230 55. 347 1. 00 18. 03 A 76. 667 59. 186 54. 143 1. 00 18. 40 A 76. 211 58. 135 56. 069 1. 00 18. 22 A 76. 246 56. 822 55. 441 1. 00 19. 90 A 76. 734 55. 752 56. 420 1. 00 22. 57 76. 819 54. 376 55. 778 1. 00 25. 97 77. 340 54. 278 54. 649 1. 00 27. 13 A 76. 372 53. 388 56. 398 1. 00 30. 03 74. 839 56. 504 54. 984 1. 00 19. 16	C 0 0 C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	5664 5665 5666 5667 5668 5669 5670 5671 5672 5674 5675 5676 5677 5678 5680 5681 5682	O ASP N PHE CA PHE CB PHE CCD PHE CD2 PHE CE2 PHE CC2 PHE CC PHE C PHE CA GLN CA GLN CB GLN CCB GLN CC	729 730 730 730 730 730 730 730 730 730 730	73. 868 56. 863 55. 649 1. 00 21. 91 A 74. 723 55. 838 53. 846 1. 00 18. 27 A 73. 416 55. 499 53. 299 1. 00 16. 06 A 72. 796 56. 734 52. 639 1. 00 14. 49 A 73. 590 57. 265 51. 480 1. 00 12. 02 A 73. 262 56. 913 50. 177 1. 00 10. 26 A 74. 691 58. 082 51. 694 1. 00 11. 55 A 74. 020 57. 364 49. 098 1. 00 10. 41 A 75. 120 58. 175 49. 317 1. 00 9. 85 A 73. 565 54. 388 52. 281 1. 00 16. 20 A 74. 675 53. 990 51. 945 1. 00 18. 49 A 72. 447 53. 883 51. 791 1. 00 17. 40 A 71. 514 51. 708 51. 208 1. 00 20. 04 A 71. 641 51. 257 52. 644 1. 00 25	N C C C C C C C C C O N C C C C O N

				(Continued)
			FIG. 4-117	
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	5684 O GLM 5685 N ALA 5686 CA ALA 5687 CB ALA 5688 C ALA 5689 O ALA 5690 N MET 5691 CA MET 5692 CB MET 5693 CG MET 5694 SD MET 5695 CE MET 5696 C MET 5697 O MET 5698 N TRP 5700 CB TRP 5700 CB TRP 5700 CB TRP 5701 CG TRP 5702 CD2 TRP 5703 CE2 TRP 5704 CE3 TRP 5705 CD1 TRP 5706 NE1 TRP 5706 NE1 TRP 5707 CZ2 TRP 5708 CZ3 TRP 5709 CH2 TRP 5709 CH2 TRP 5710 C TRP 5711 O TRP 5711 O TRP 5712 N TYR 5713 CA TYR 5713 CA TYR 5714 CB TYR 5715 CG TYR 5716 CD1 TYR 5717 CE1 TYR 5717 CE1 TYR 5718 CD2 TYR 5719 CE2 TYR 5719 CE2 TYR 5719 CE2 TYR 5719 CE2 TYR 5720 CZ TYR	732 732 732 732 732 733 733 733 733 733	FIG. 4 - 117 71.160 54.191 49.355 1.00 17.02 A 72.802 52.962 48.421 1.00 14.78 A 72.510 53.444 47.088 1.00 15.21 A 73.588 54.409 46.626 1.00 15.17 A 72.419 52.282 46.131 1.00 15.21 A 71.737 52.504 45.019 1.00 14.57 A 71.599 51.483 44.008 1.00 14.57 A 71.599 51.483 44.008 1.00 14.86 A 70.490 50.499 44.383 1.00 15.14 A 70.288 49.386 43.353 1.00 18.04 A 71.814 48.476 42.961 1.00 22.04 A 71.892 47.307 44.310 1.00 17.75 A 71.283 52.153 42.683 1.00 14.93 A 70.317 52.915 42.574 1.00 13.98 A 72.113 51.884 41.680 1.00 13.82 A 71.890 52.447 40.356 1.00 13.82 A 71.890 52.447 40.356 1.00 13.13 A 73.173 53.117 39.827 1.00 10.39 A 74.187 52.159 39.267 1.00 8.77 A 75.398 51.726 39.894 1.00 7.74 A 75.984 50.757 39.053 1.00 9.97 A 76.045 52.062 41.087 1.00 8.70 A 77.183 50.119 39.369 1.00 10.56 A 77.183 50.119 39.369 1.00 9.94 A 77.238 51.428 41.400 1.00 9.32 77.793 50.468 40.545 1.00 9.49 A 71.480 51.291 39.445 1.00 12.87 A 77.183 50.19 39.369 1.00 9.94 A 77.238 51.428 41.400 1.00 9.32 77.793 50.468 40.545 1.00 9.49 A 71.480 51.291 39.445 1.00 14.06 A 71.903 50.155 39.653 1.00 13.91 A 70.635 51.570 38.461 1.00 15.51 A 68.300 49.439 38.709 1.00 14.76 A 68.619 48.081 38.708 1.00 14.45 A 68.360 47.278 39.816 1.00 14.33 A 67.696 49.971 39.848 1.00 15.84 A 67.772 47.835 40.938 1.00 14.52 A 67.772 47.835 40.938 1.00 15.53 A	(Continued) O N C C C C C C C C C C C C C C C C C
ATOM	5720 CZ TYR 5721 OH TYR		67 779 47 995 40 000 1 00 10 00	C
ATOM	5722 C TYR	735	70. 685 50. 966 36. 104 1. 00 16. 31 A	C C
ATOM ATOM	5723 O TYR 5724 N THR	735 736	70. 103 51. 858 35. 466 1. 00 15. 82 A	0
ATOM	5725 CA THR	736	71. 763 50. 330 35. 654 1. 00 15. 44 A 72. 361 50. 608 34. 353 1. 00 15. 13 A	N C
ATOM	5726 CB THR	736	73. 491 49. 602 34. 030 1. 00 14. 68 A	C
ATOM ATOM	5727 OG1 THR 5728 CG2 THR	736	74. 470 49. 614 35. 076 1. 00 15. 48 A	ŏ
ATOM	5728 CG2 THR 5729 C THR	736 736	74. 156 49. 961 32. 713 1. 00 14. 72 A 71. 365 50. 549 33. 206 1. 00 15. 41 A	C
ATOM	5730 0 THR	736	71. 365 50. 549 33. 206 1. 00 15. 41 A 70. 650 49. 560 33. 044 1. 00 16. 44 A	C 0
ATOM	5731 N ASP	737	71. 335 51. 614 32. 414 1. 00 15. 92 A	N N
ATOM	5732 CA ASP	737	70. 475 51. 719 31. 238 1. 00 16. 48 A	Ċ

						٠.				(Continued)
					FI	G. 4-	118			(Continued)
	5500	an	4.00	707				. 1 00 15 00		
ATOM	5733	CB	ASP	737	70. 884		30. 200	1.00 15.90	A	C
ATOM	5734	CG	ASP	737	72. 232		29. 574	1.00 20.37	A	C
ATOM	5735		ASP	737	72.679		28. 747	1.00 24.29	A	0
MOTA	5736		ASP	737	72. 847		29. 895	1.00 18.74	A	0
ATOM	5737	C	ASP	737	68.974		31.467	1.00 17.71	A	C
ATOM	5738	0	ASP	737	68. 205		30. 515	1.00 18.86	A	0
ATOM	5739	N	GLU	738	68.553		32. 722	1.00 18.39	A	N
ATOM	5740	CA	GLU	738	67. 135			1.00 19.00	A	C .
ATOM	5741	CB	GLU	738	66. 909		34. 407	1.00 20.24	A	C
ATOM	5742	CG	GLU	738	66. 904		34. 380	1.00 20.93	A	C
ATOM	5743	CD	GLU	738	65. 741		33. 565	1.00 24.58	A	C
ATOM	5744		GLU	738	64. 588		33. 878	1.00 27.21	A	0
ATOM	5745		GLU	738	65. 970		32.611	1.00 26.16	A	0
ATOM	5746	C	GLU	738	66. 624		33. 025	1.00 19.38	A	C
ATOM	5747	0	GLU	738	67. 327		33. 461	1.00 20.83	A	0
ATOM	5748	N	ASP	739	65. 414		32. 525	1.00 18.55	A	N
ATOM	5749	CA	ASP	739	64. 892		32. 493	1.00 17.49	A	C
ATOM	5750	CB	ASP	739	64.074		31. 222	1.00 18.32	A	C
ATOM	5751	CG	ASP	739	62. 689			1.00 21.44	A	C
ATOM	5752		ASP	739	61.995		30. 257	1.00 24.73	A	0
ATOM	5753		ASP	739	62. 285		32. 358	1.00 21.35	A	0
ATOM	5754	C	ASP	739	64.088		33.750	1.00 17.35	A	C
ATOM	5755	0	ASP	739	64. 191		34. 762	1.00 15.74	A	0
ATOM	5756 5757	N	HIS	740 740	63. 291		33. 687	1.00 16.96	A	N
ATOM ATOM	5757 5750	CA	HIS				34. 842	1.00 18.24	A	C
ATOM	5758 5759	CB CG	HIS HIS	740 740	61.746		34.511	1.00 16.88	A	C
ATOM	5760		HIS	740 740	61.145			1.00 17.57	A	C
ATOM	5761		HIS	740	59. 883		35.961	1.00 16.26	A	C
ATOM	5762		HIS	740	61.881		36. 837	1.00 17.31	A	N
ATOM	5763		HIS	740 740	61. 097 59. 880		37. 732 37. 224	1.00 18.51	A	C
ATOM	5764	C	HIS	740	61. 557			1.00 17.94	A	N
ATOM	5765	Ö	HIS	740	61. 191	55. 449 55. 539	35. 426 36. 599	1.00 19.90 1.00 20.00	A	C
ATOM	5766	N	GLY	741	61.151	54. 481	34.614	1.00 20.00	A	0 N
ATOM	5767	CA	GLY	741	60. 216		35. 084	1.00 19.40	A	N .
ATOM	5768		GLY	741	60. 849			1.00 10.02	A	C
ATOM	5769	Õ	GLY	741	60.165		36. 237		A	C
ATOM	5770	N	ILE	742	62. 145		35. 368	1.00 22.79 1.00 19.61	A	0 N
ATOM	5771	CA	ILE	742	62. 854		35. 821	1.00 19.01	A	N C
ATOM	5772	CB	ILE	742	63. 273	50. 981	37. 294		A	C
ATOM	5773		ILE	742	64. 279	49. 917	37. 638	1.00 14.46 1.00 14.37	A	C
ATOM	5774		ILE	742	63. 865		37. 540	1.00 14.37	A A	C C
ATOM	5775		ILE	742	64. 540		38. 887	1.00 13.43	A	C ·
ATOM	5776	C	ILE	742	61.907		35. 676	1.00 9.55	A A	C
ATOM	5777	Õ	ILE	742	61.805	48. 825	36. 571	1.00 19.11	A	0
ATOM	5778	Ň	ALA	743	61. 217	49. 594	34. 534	1.00 10.31	A	N N
ATOM	5779	CA	ALA	743	60. 246	48. 538	34. 268	1.00 20.10	A	C
ATOM	5780	CB	ALA	743	59. 004	49. 141	33. 630	1.00 19.65	A	C
ATOM	5781	Č	ALA	743	60.717	47. 350	33. 430	1.00 20.08	Ä	C
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ATOM 5821 CD GLN 749 61.618 39.190 37.757 1.00 20.87 A C ATOM 5822 OE1 GLN 749 62.047 38.187 38.316 1.00 22.37 A O ATOM 5823 NE2 GLN 749 61.415 39.249 36.447 1.00 20.00 A N ATOM 5824 C GLN 749 63.416 42.524 41.008 1.00 19.07 A C ATOM 5825 O GLN 749 63.335 42.388 42.231 1.00 17.88 A O ATOM 5826 N HIS 750 64.508 42.972 40.399 1.00 18.97 A N ATOM 5827 CA HIS 750 65.707 43.275 41.160 1.00 16.68 A C ATOM 5828 CB HIS 750 66.871 43.597 40.226 1.00 14.65 A C ATOM 5829 CG HIS 750 68.208 43.496 40.889 1.00 13.97 A C						61.29								
ATOM 5823 NE2 GLN 749 61.415 39.249 36.447 1.00 20.00 A N ATOM 5824 C GLN 749 63.416 42.524 41.008 1.00 19.07 A C ATOM 5825 O GLN 749 63.335 42.388 42.231 1.00 17.88 A O ATOM 5826 N HIS 750 64.508 42.972 40.399 1.00 18.97 A N ATOM 5827 CA HIS 750 65.707 43.275 41.160 1.00 16.68 A C ATOM 5828 CB HIS 750 66.871 43.597 40.226 1.00 14.65 A C ATOM 5829 CG HIS 750 68.208 43.496 40.889 1.00 13.97 A C								190		1.00	20.87			
ATOM 5824 C GLN 749 63.416 42.524 41.008 1.00 19.07 A C ATOM 5825 O GLN 749 63.335 42.388 42.231 1.00 17.88 A O ATOM 5826 N HIS 750 64.508 42.972 40.399 1.00 18.97 A N ATOM 5827 CA HIS 750 65.707 43.275 41.160 1.00 16.68 A C ATOM 5828 CB HIS 750 66.871 43.597 40.226 1.00 14.65 A C ATOM 5829 CG HIS 750 68.208 43.496 40.889 1.00 13.97 A C												Α	0	
ATOM 5825 O GLN 749 63.335 42.388 42.231 1.00 17.88 A O ATOM 5826 N HIS 750 64.508 42.972 40.399 1.00 18.97 A N ATOM 5827 CA HIS 750 65.707 43.275 41.160 1.00 16.68 A C ATOM 5828 CB HIS 750 66.871 43.597 40.226 1.00 14.65 A C ATOM 5829 CG HIS 750 68.208 43.496 40.889 1.00 13.97 A C														
ATOM 5826 N HIS 750 64.508 42.972 40.399 1.00 18.97 A N ATOM 5827 CA HIS 750 65.707 43.275 41.160 1.00 16.68 A C ATOM 5828 CB HIS 750 66.871 43.597 40.226 1.00 14.65 A C ATOM 5829 CG HIS 750 68.208 43.496 40.889 1.00 13.97 A C														
ATOM 5827 CA HIS 750 65.707 43.275 41.160 1.00 16.68 A C ATOM 5828 CB HIS 750 66.871 43.597 40.226 1.00 14.65 A C ATOM 5829 CG HIS 750 68.208 43.496 40.889 1.00 13.97 A C														
ATOM 5828 CB HIS 750 66.871 43.597 40.226 1.00 14.65 A C ATOM 5829 CG HIS 750 68.208 43.496 40.889 1.00 13.97 A C														
ATOM 5829 CG HIS 750 68.208 43.496 40.889 1.00 13.97 A C													Ü	
	ATOM	5830			750				40. 749			A	C	

		(Continued)				
				FIG. 4-120		
ATOM ATOM	5831 5832	ND1 HIS CE1 HIS	750 750	68.615 44.365 41.877 1.00 13.54 69.804 44.000 42.320 1.00 12.57	A	N
ATOM	5833	NE2 HIS	750	69.804 44.000 42.320 1.00 12.57 70.185 42.927 41.653 1.00 12.04	A	C
ATOM	5834	C HIS	750	65.529 44.400 42.157 1.00 17.33	A A	N C
ATOM	5835	0 HIS	750	65. 945 44. 277 43. 309 1. 00 18. 09	A	Õ
ATOM	5836	N ILE	751	64.899 45.490 41.726 1.00 17.03	A	Ň
ATOM	5837	CA ILE	751	64.704 46.632 42.604 1.00 15.90	Ä	Ĉ
ATOM	5838	CB ILE	751	64. 206 47. 849 41. 805 1. 00 17. 60	Ā	č
ATOM	5839	CG2 ILE	751	62.893 47.504 41.088 1.00 16.17	A	C
ATOM	5840	CG1 ILE	751	64. 065 49. 058 42. 736 1. 00 15. 94	Α	C
ATOM	5841	CD1 ILE	751	63. 684 50. 332 42. 017 1. 00 12. 51	A	C
ATOM ATOM	5842	C ILE	751	63. 751 46. 341 43. 767 1. 00 16. 09	A	Ċ
ATOM	5843 5844	0 ILE N TYR	751 752	64.062 46.632 44.919 1.00 16.37	A	0
ATOM	5845	CA TYR	752 752	62.596 45.759 43.480 1.00 16.32 61.651 45.449 44.551 1.00 16.16	A	N
ATOM	5846	CR TYR	752	61.651 45.449 44.551 1.00 16.16 60.323 44.967 43.968 1.00 13.79	A	C
ATOM	5847	CG TYR	752	59. 443 46. 126 43. 593 1. 00 12. 59	A A	C C
ATOM	5848	CD1 TYR	752	58.840 46.899 44.580 1.00 11.61	A	C
ATOM	5849	CE1 TYR	752	58.102 48.026 44.258 1.00 9.67	A	C
ATOM	5850	CD2 TYR	752	59. 279 46. 510 42. 260 1. 00 12. 75	A	č
ATOM	5851	CE2 TYR	752	58. 543 47. 644 41. 930 1. 00 10. 28	Ä	C C
ATOM	5852	CZ TYR	752	57. 964 48. 395 42. 940 1. 00 9. 02	Α	C
ATOM	5853	OH TYR	752	57. 278 49. 542 42. 642 1. 00 12. 10	Α	0
ATOM ATOM	5854	C TYR	752	62. 226 44. 429 45. 522 1. 00 16. 42	Α	C.
ATOM	5855 5856	O TYR N THR	752	61. 927 44. 467 46. 719 1. 00 16. 42	A	0
ATOM	5857	CA THR	753 753	63. 056 43. 526 45. 004 1. 00 15. 74 63. 700 42. 521 45. 835 1. 00 16. 30	A	N
ATOM	5858	CB THR	753		A	C
ATOM	5859	OG1 THR	753	64. 502 41. 510 44. 985 1. 00 15. 57 63. 601 40. 677 44. 253 1. 00 15. 74	A	C
ATOM	5860	CG2 THR	753	65. 385 40. 641 45. 870 1. 00 10. 01	A A	0 C
ATOM	5861	C THR	753	64. 678 43. 240 46. 758 1. 00 18. 17	A	C
ATOM	5862	0 THR	753	64. 788 42. 923 47. 941 1. 00 19. 02	A	. 0
ATOM	5863	N HIS	754	65. 388 44. 215 46. 199 1. 00 18. 78	Ä	Ň
ATOM	5864	CA HIS	754	66. 363 44. 972 46. 959 1. 00 18. 90	Α	C
ATOM	5865	CB HIS	754	67. 189 45. 857 46. 023 1. 00 19. 13	Α	C
ATOM	5866 5967	CG HIS	754 754	68. 449 46. 379 46. 644 1. 00 19. 62	Α	C
ATOM ATOM	5867 5868	CD2 HIS	754 754	68. 786 47. 619 47. 070 1. 00 18. 70	A	C
ATOM	5869	CE1 HIS	754 754	69. 539 45. 576 46. 904 1. 00 18. 44 70. 493 46. 298 47. 462 1. 00 17. 52	A	N
ATOM	5870	NE2 HIS	754		A	C
ATOM	5871	C HIS	754	70.062 47.541 47.574 1.00 19.51 65.663 45.828 48.007 1.00 19.38	A A	N C
ATOM	5872	0 HIS	754	66. 088 45. 876 49. 158 1. 00 19. 63	A	0
ATOM	5873	N MET	755	64. 589 46. 502 47. 615 1. 00 18. 83	A	N
ATOM	5874	CA MET	755	63. 854 47. 342 48. 558 1. 00 19. 68	Ä	Č
ATOM	5875	CB MET	755	62. 758 48. 136 47. 839 1. 00 16. 86	Ä	Č
ATOM	5876	CG MET	755	63. 283 49. 173 46. 876 1. 00 16. 00	Α	С
ATOM	5877 5070	SD MET	755 755	62.016 50.314 46.309 1.00 20.78	Α	S
ATOM ATOM	5878 5879	CE MET C MET	755 755	61.100 49.270 45.200 1.00 15.61	A	C
ATOR	0013	O 14117.1	755	63. 232 46. 506 49. 676 1. 00 20. 27	A	С

					<u>.</u>					(Continued)
					FIC	3.4-	122	}		(COHOLING)
ATOM ATOM ATOM	5929 5930 5931	CD OE I NE 2		761 761 761	68. 759 68. 487 69. 177	46. 893 47. 969 46. 811	58. 283 57. 739 59. 544	1.00 43.62	A A A	C O .N
ATOM ATOM	5932 5933	C 0	GLN GLN	761 761	65. 819 66. 064	46. 251 46. 149	58. 701 59. 898	1.00 32.55	A A	0 C.
ATOM	5934	N	CYS	762	65. 276	47. 337	58. 161	1.00 32.03	Α	N
ATOM ATOM	5935 5936	CA C	CYS CYS	762 762	64. 945 63. 888	48. 513 48. 216	58. 953 60. 023		A A	C
ATOM ATOM	5937 5938	O CB	CYS CYS	762 762	63. 892 64. 470	48. 830 49. 643	61. 087 58. 025		A	0
ATOM	5939	SG	CYS	762	63.606	51.029	58.843	1.00 40.21	A A	C S
ATOM ATOM	5940 5941	N CA	PHE PHE	763 763	62. 993 61. 948	47. 271 46. 907	59. 742 60. 694	1.00 32.59 1.00 34.25	A A	N C
ATOM ATOM	5942 5943	CB CG	PHE PHE	763 763	60. 618 59. 919	46. 647 47. 892	59. 981 59. 525	1.00 31.61	Α	C
ATOM	5944	CD1	PHE	763 .	60.371	49. 148	59.923	1.00 30.04 1.00 29.45	A A	C C
ATOM ATOM	5945 5946		PHE PHE	763 763	58.800 59.718	47. 808 50. 300	58. 703 59. 510	1.00 28.65 1.00 29.27	A A	C C
ATOM ATOM	5947 5948	CE2	PHE	763 763	58. 139 58. 598	48. 951 50. 202	58. 284 58. 688	1.00 28.76 1.00 30.54	Α	C C
ATOM	5949	C	PHE	763	62.293	45.688	61.535	1.00 36.77	A A	С
ATOM ATOM	5950 5951	O N	PHE SER	763 764	61. 499 63. 463	45. 276 45. 102	62. 381 61. 290	1.00 36.29 1.00 39.62	A A	0 N
ATOM ATOM	5952 5953	CA CB	SER SER	764 764	63. 907 65. 356	43. 941 43. 598	62. 052 61. 701	1.00 43.05 1.00 44.44	Α	С
ATOM	5954	0G	SER	764	66. 215	44.709	61.913	1.00 48.06	A A	C 0
ATOM ATOM	5955 5956	C 0	SER SER	764 764	63. 799 64. 195	44. 314 45. 412	63. 522 63. 916	1.00 45.02 1.00 44.75	A A	C 0
ATOM ATOM	5957 5958	N CA	LEU LEU	765 765	63. 264 63. 092	43. 412 43. 716	64. 335 65. 747	1.00 48.04 1.00 51.59	Α	N .
ATOM	5959	. CB	LEU	765	61.624	44.067	66.017	1.00 50.97	A A	C C
ATOM ATOM	5960 5961		LEU LEU	765 765		44. 846 46. 215	67. 299 67. 221	1.00 50.79 1.00 50.85	A A	C C
ATOM ATOM	5962 5963	CD2 C	LEU LEU	765 765	59. 834 63. 533	44. 996 42. 588	67. 481 66. 676	1.00 50.72 1.00 54.72	A A	C C
ATOM ATOM	5964 5965	0 N	LEU	765	62.866	41.557	66.779	1.00 55.73	A	0
ATOM	5966	CD	PRO PRO	766 766	65. 545	42. 776 43. 960	67. 372 67. 317	1.00 57.13 1.00 57.88	A A	N C
ATOM ATOM	5967 5968	CA CB	PRO PRO	766 766		41. 775 42. 309	68. 301 68. 604	1.00 58.61 1.00 58.49	A A	C C
ATOM ATOM	5969 5970	CG C	PRO PRO	766 766	66.386	43. 797 41. 639	68. 568 69. 565	1.00 58.47	Α	C
ATOM	5971	0	PR0	766	63. 341	42.370	69.681	1.00 60.07 1.00 60.04	A A	C 0
ATOM TER	5972 5973	UXT	PRO PRO	766 766	64. 711	40. 805	70. 427	1.00 61.88	A A	0
ATOM ATOM	5974 5975	CB CG	ASP ASP	38 38		45. 132 46. 047	76. 302 75. 698	1.00 32.66 1.00 32.61	В	C
ATOM ATOM	5976 5977	0D1	ASP	38	96. 905	47. 269	75. 977	1.00 30.88	B B	C 0
VION	0311	OD2	uor	38	97. 816	45.544	74. 942	1.00 31.65	В	0

					FIC	G. 4-	123			(Continued)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	5978 5979 5980 5981 5982 5983 5984 5985 5986 5987 5992 5993 5994 5995 5996 6001 6002 6003 6004 6005 6006 6007 6008 6009 6010	O N CA N CA CB CC CD N CA CB CC CD N CA CB CC CD N CA CB CC	ARG ARG LYS	38 38 38 39 39 39 39 40 40 40 40 40 40 41 41 41 41 41 41 42 42 42 42 42	94. 533 93. 521 94. 842 95. 507 94. 844 93. 974 94. 048 95. 362 94. 289 93. 615 95. 685 97. 004 98. 228 99. 404 100. 260 101. 247 100. 134 94. 604 93. 881 94. 494 93. 518 93. 386 94. 699 94. 505 94. 374 93. 307 94. 028 95. 231 93. 118 93. 518 92. 454 91. 257 92. 128	46. 724 46. 648 44. 428 45. 557 47. 807 48. 982 49. 652 50. 119 50. 017 51. 049 49. 755 50. 686 50. 257 50. 429 49. 917 48. 461 46. 497 50. 757 49. 793 51. 907 52. 076 53. 556 54. 209 55. 663 55. 779 54. 922 51. 294 51. 072 50. 130 49. 083 49. 753 48. 129	77. 638 76. 938 78. 423 77. 717 78. 344 78. 372 79. 741 80. 003 77. 220 76. 499 75. 442 74. 788 75. 670 74. 969 74. 728 73. 361 73. 806 74. 376 74. 150 73. 725 72. 658 72. 274 71. 365 69. 840 69. 251 71. 458 71. 324 70. 595 69. 399 68. 959 68. 540 70. 101	1. 00 31. 81 1. 00 32. 54 1. 00 32. 95 1. 00 32. 96 1. 00 31. 40 1. 00 30. 28 1. 00 31. 88 1. 00 34. 53 1. 00 29. 15 1. 00 30. 29 1. 00 26. 40 1. 00 24. 29 1. 00 21. 38 1. 00 21. 28 1. 00 22. 73 1. 00 22. 52 1. 00 22. 23 1. 00 22. 23 1. 00 23. 29 1. 00 23. 29 1. 00 23. 29 1. 00 23. 29 1. 00 23. 55 1. 00 24. 31 1. 00 25. 29 1. 00 28. 84 1. 00 28. 95 1. 00 27. 49 1. 00 24. 69 1. 00 22. 69 1. 00 22. 69 1. 00 21. 91 1. 00 20. 28	B B B B B B B B B B B B B B B B B B B	CONCNCCOCONCCCNCNNCONCCCCCNCONCCOC
ATOM ATOM ATOM	6013 6014 6015	C '	THR THR TYR	42 42 43	93. 641 93. 386 94. 045	51.178 52.363 50.750	68. 304 68. 541 67. 116	1.00 22.33 1.00 23.36 1.00 20.55	B B B	C O N
ATOM ATOM ATOM	6016 6017 6018	CA CB CCG	TYR TYR TYR	43 43 43	94. 158 95. 233 95. 516	51. 662 51. 153 52. 062	65. 986 65. 020 63. 853	1.00 19.19 1.00 20.32 1.00 19.92	B B B	C C C
ATOM ATOM ATOM ATOM	6019 6020 6021 6022	CD1 1 CE1 1 CD2 1 CE2 1	TYR TYR	43 43 43 43	94. 888 95. 133 96. 403 96. 655	51. 863 52. 694 53. 126	62. 629 61. 546 63. 970	1.00 22.19 1.00 21.23 1.00 21.09	B B B	C C C
ATOM ATOM ATOM ATOM	6023 6024 6025 6026	CZ 1 OH 1 C 3	TYR TYR TYR TYR TYR	43 43 43 43	96. 013 96. 247 92. 770	53. 972 53. 742 54. 553 51. 631	62. 891 61. 682 60. 600 65. 349	1.00 21.69 1.00 22.25 1.00 25.44 1.00 18.52	B B B	C C O C
111 Oill	0020	υ J	1111	40	92. 396	50. 640	64. 725	1.00 17.41	В	0

										(Continued)
					FI	G. 4-	124			
ATOM	6027		THR	44	92.007	52.709	65.532	1.00 17.70	В	N
ATOM	6028		THR	44	90.633	52.802	65.019	1.00 18.55	В	C
ATOM	6029		THR	44	89.762	53. 748	65. 877	1.00 16.45	В	C
ATOM	6030		THR	44	90. 195	55. 096	65.676	1.00 16.93	В	0
ATOM	6031	CG2		44	89. 875	53.409	67.346	1.00 14.45	В	C
ATOM	6032		THR	44	90. 521	53. 310	63. 593	1.00 19.62	В	C
ATOM	6033		THR	44	91.511	53. 741	62.992	1.00 21.89	B B	0
ATOM ATOM	6034 6035		LEU LEU	45 45	89. 296 89. 026	53. 277 53. 749	63.067 61.713	1.00 19.06 1.00 18.74	В	N C
ATOM	6036		LEU	45	87.570	53. 489	61.327	1.00 17.33	В	C
ATOM	6037		LEU	45	87. 163	54. 032	59.952	1.00 17.35	В	č
ATOM	6038	CD1		45	88. 050	53. 417	58. 873	1.00 15.87	В	č
ATOM	6039	CD2		45	85.698	53. 720	59.681	1.00 16.27	B	č
ATOM	6040		LEU	45	89. 300	55. 240	61.638	1.00 19.82	B	C C
ATOM	6041		LEU	45	89.827	55.743	60.638	1.00 21.32	В	Ŏ
ATOM	6042	N	THR	46	88. 948	55.945	62.707	1.00 19.07	В	N
ATOM	6043	CA	THR	46	89. 156	57. 382	62.760	1.00 20.55	В	С
ATOM	6044		THR	46	88. 550	57. 988	64.038	1.00 21.32	В	C
ATOM	6045		THR	46	87. 148	57.700	64.083	1.00 21.56	В	0
ATOM	6046	CG2		46	88. 745	59. 497	64.053	1.00 20.61	В	C
ATOM	6047		THR	46	90.634	57. 749	62.694	1.00 21.16	В	C
ATOM	6048		THR	46	90. 999	58. 759	62.092	1.00 21.06	В	0
ATOM	6049		ASP	47	91. 491	56.945	63.313	1.00 21.00	В	N
ATOM ATOM	6050 6051		ASP ASP	47 47	92. 910 93. 731	57. 253 56. 273	63. 262	1.00 22.97	В	C
ATOM	6052		asp ASP	47	93. 365	56. 322	64.110 65.578	1.00 25.34 1.00 27.23	B B	C C
ATOM	6053	0D1		47	93. 116	57. 430	66. 105	1.00 26.32	В	0
ATOM	6054	0D2		47	93. 339	55. 244	66. 208	1.00 20.32	В	0
ATOM	6055		ASP	47	93. 357	57. 178	61.810	1.00 22.85	В	Č
ATOM	6056		ASP	47	94. 057	58.065	61.320	1.00 24.15	B	ő
ATOM	6057		TYR	48	92. 951	56.124	61.114	1.00 20.92	B	Ň
ATOM	6058	CA	TYR	48	93. 332	55.998	59.720	1.00 21.40	В	C
ATOM	6059		TYR	48	92.823	54.676	59.136	1.00 19.45	В	C
ATOM	6060		TYR	48	92.867	54.612	57.624	1.00 18.60	В	С
ATOM	6061		TYR	48	94.062	54. 787	56.927	1.00 18.00	В	С
ATOM	6062	CE1		48	94. 098	54. 734	55. 531	1.00 16.57	В	C
ATOM	6063	CD2		48	91.702	54. 383	56. 885	1.00 21.30	В	C
ATOM	6064	CE2		48	91.726	54. 329	55. 489	1.00 19.50	В	C
ATOM	6065		TYR	48	92. 925	54. 503	54. 822	1.00 18.43	В	C
ATOM ATOM	6066 6067		TYR TYR	48 48	92. 942	54. 434	53. 452	1.00 18.40	В	0
ATOM	6068		TYR	48 48	92. 795 93. 547	57. 170 57. 853	58. 899 58. 207	1.00 21.85 1.00 21.92	B B	C
ATOM	6069		LEU	49	91. 497	57.416	58. 996	1.00 21.32	В	O N
ATOM	6070		LEU	49	90. 885	58. 485	58. 223	1.00 26.78	В	C
ATOM	6071		LEU	49	89.359	58. 437	58. 381	1.00 28.14	В	č
ATOM	6072		LEU	49	88. 688	57. 157	57. 872	1.00 28.75	B	č
ATOM	6073	CD1		49	87. 188	57. 305	57.980	1.00 28.04	$\bar{\mathbf{B}}$	č
ATOM	6074	CD2	LEU	49	89.094	56.889	56.420	1.00 28.45	В	C
ATOM	6075	C	LEU	49	91.391	59.886	58. 544	1.00 28.33	В	С

					(Continued)
				FIG. 4-126	
ATOM	6125		55	104. 959 58. 926 59. 515 1. 00 24. 45 B	С
ATOM	6126		55	105.025 57.911 58.382 1.00 22.51 B	C
ATOM	6127		55	104. 335 56. 575 58. 631 1. 00 23. 77 B	C
ATOM ATOM	6128 6129		55	104. 287 55. 792 57. 336 1. 00 23. 51 B	C
ATOM	6130		55 55	105.083 55.796 59.703 1.00 22.83 B	C
ATOM	6131		55	105. 773 60. 161 59. 135 1. 00 24. 19 B 105. 428 60. 867 58. 187 1. 00 23. 47 B	C
ATOM	6132		56	100 004 00 100 00	0
ATOM	6133		56	107 001 01 000 00	N
ATOM	6134		56	107. 631 61. 603 59. 532 1. 00 23. 81 B 108. 536 62. 028 60. 680 1. 00 25. 76 B	C C
ATOM	6135		56	107. 850 62. 922 61. 697 1. 00 29. 15 B	Č
ATOM	6136		56	108.868 63.560 62.638 1.00 31.22 B	Č
ATOM	6137	CE LYS	56	108. 225 64. 593 63. 548 1. 00 32. 59 B	Č
ATOM-	6138		56	109. 235 65. 233 64. 439 1. 00 34. 54 B	Ň
ATOM	6139	C LYS	56	108. 458 61. 196 58. 330 1. 00 23. 35 B	Č
ATOM	6140	0 LYS	56	108. 833 60. 035 58. 186 1. 00 23. 24 B	ŏ
ATOM	6141	N LEU	57	108.717 62.162 57.462 1.00 22.99 B	Ň
ATOM	6142	CA LEU	57	109. 477 61. 945 56. 247 1. 00 22. 29 B	С
ATOM	6143	CB LEU	57	108. 612 62. 292 55. 040 1. 00 23. 21 B	C
ATOM ATOM	6144	CG LEU	57	107. 169 61. 794 55. 037 1. 00 23. 82 B	С
ATOM	6145 6146	CD1 LEU CD2 LEU	57 57	106. 440 62. 380 53. 841 1. 00 24. 84 B	C .
ATOM	6147	CDZ LEU	57 57	107. 145 60. 278 54. 992 1. 00 25. 36 B	C
ATOM	6148	0 LEU	57	110. 681 62. 870 56. 256 1. 00 22. 04 B 110. 888 63. 628 57. 202 1. 00 22. 65 B	C
ATOM	6149	N TYR	58	111 100 00 000 ==	0
ATOM	6150	CA TYR	58	110 004 00 004	N
ATOM	6151	CB TYR	58	110 001 00 000	C
ATOM	6152	CG TYR	58	113.834 63.089 55.795 1.00 19.94 B 114.933 64.099 56.008 1.00 18.95 B	C C
ATOM	6153	CD1 TYR	58	115.845 64.392 54.998 1.00 19.13 B	C
ATOM	6154	CE1 TYR	58	116. 816 65. 380 55. 165 1. 00 18. 92 B	Č
ATOM	6155	CD2 TYR	58	115.022 64.816 57.201 1.00 19.88 B	č
ATOM	6156	CE2 TYR	58	115. 987 65. 807 57. 378 1. 00 19. 69 B	č
ATOM	6157	CZ TYR	58	116.877 66.086 56.355 1.00 19.43 B	č
ATOM	6158	OH TYR	58	117.804 67.092 56.508 1.00 19.58 B	Ö
ATOM	6159	C TYR	58	112.917 63.819 53.590 1.00 20.38 B	С
ATOM ATOM	6160	O TYR	58	113. 861 63. 223 53. 079 1. 00 20. 32 B	0
ATOM	6161 6162		59 50	112.085 64.604 52.909 1.00 21.33 B	N
ATOM	6163	CA SER CB SER	59 59	112. 245 64. 839 51. 479 1. 00 22. 11 B	C
ATOM	6164	OG SER	59	110.920 65.275 50.852 1.00 21.08 B 109.985 64.212 50.843 1.00 24.94 R	C
ATOM	6165	C SER	59		0
ATOM	6166	0 SER	59	110 000 4- 11	C .
ATOM	6167	N LEU	60	111 101 0= 11	0
ATOM	6168	CA LEU	60	114. 404 65. 485 50. 602 1. 00 21. 76 B 115. 449 66. 436 50. 273 1. 00 23. 50 B	N C
ATOM	6169	CB LEU	60	116.752 66.062 50.986 1.00 22.27 B	C
ATOM	6170	CG LEU	60	117. 406 64. 737 50. 612 1. 00 18. 62 B	C
ATOM	6171	CD1 LEU	60	118.176 64.900 49.320 1.00 17.05 B	Č
ATOM	6172	CD2 LEU	60	118.338 64.313 51.724 1.00 19.95 B	C
ATOM	6173	C LEU	60	115.656 66.478 48.762 1.00 24.93 B	Č
				SUBSTITUTE SHEET (RULE 26)	

						(Continued)
			FIG. 4	1 - 1 2 7		
ATOM ATOM ATOM ATOM ATOM	6175 N 6176 CA 6177 CB	LEU 60 ARG 61 ARG 61 ARG 61 ARG 61	115.176 65.6 116.375 67.4 116.634 67.6 115.693 68.3 115.779 68.9	495 48.302 1.00 559 46.881 1.00 728 46.329 1.00	D 23. 79 B D 26. 02 B D 27. 11 B D 32. 13 B D 38. 27 B	O N C C C
ATOM ATOM ATOM ATOM	6180 NE	ARG 61 ARG 61 ARG 61 ARG 61	115.002 70.2 114.937 70.5 114.298 71.5 113.671 72.4	506 43.063 1.00 543 42.525 1.00	0 41.78 B 0 46.51 B 0 49.47 B 0 48.74 B	C N C N
ATOM ATOM ATOM	6183 NH2 6184 C 6185 O	ARG 61 ARG 61 ARG 61	114. 266 71. 6 118. 080 68. 0 118. 475 69. 1	393 41.205 1.00 175 46.676 1.00 80 47.052 1.00	0 50.07 B 0 26.01 B 0 26.36 B	N C O
ATOM ATOM ATOM ATOM	6187 CA 6188 CB 6189 CG	TRP 62 TRP 62 TRP 62 TRP 62	118.877 67.1 120.282 67.4 121.024 66.2 121.095 65.1	88 45.846 1.00 44 45.355 1.00 45 46.365 1.00	25. 15 B 24. 48 B 20. 04 B 18. 16 B	Ñ C C C
ATOM ATOM ATOM ATOM	6190 CD2 6191 CE2 6192 CE3 6193 CD1	TRP 62 TRP 62	121. 954 65. 0 121. 639 63. 9 122. 956 65. 9 120. 315 64. 0	10 48.215 1.00 32 48.007 1.00	14.54 B 15.18 B 12.41 B 17.39 B	C C C
ATOM ATOM ATOM ATOM	6194 NE1 6195 CZ2 6196 CZ3 6197 CH2	TRP 62 TRP 62 TRP 62	120. 639 63. 2 122. 292 63. 5 123. 606 65. 5 123. 271 64. 3	72 47.528 1.00 46 49.397 1.00 75 49.183 1.00	15.77 B 16.35 B 14.94 B 16.25 B	N C C C
ATOM ATOM ATOM	6198 C 6199 O 6200 N	TRP 62 TRP 62 ILE 63	120. 401 68. 5 119. 863 68. 4 121. 088 69. 6	88 44.798 1.00 57 43.698 1.00 75 45.135 1.00	26. 73 B 27. 86 B 27. 97 B	C O N
ATOM ATOM ATOM ATOM	6202 CB 6203 CG2 6204 CG1	ILE 63	121. 265 70. 7 120. 947 72. 1 119. 476 72. 1 121. 830 72. 3	30 44.803 1.00 93 45.169 1.00 72 46.027 1.00	29. 02 B 29. 64 B 30. 36 B 30. 01 B	C C C
ATOM ATOM ATOM ATOM	6207 0	ILE 63 ILE 63 ILE 63 SER 64	121. 542 73. 6 122. 693 70. 7 123. 062 71. 6 123. 485 69. 8	71 43.657 1.00 09 42.835 1.00	27. 88 B 30. 19 B 31. 12 B 30. 03 B	C C O N
ATOM ATOM ATOM ATOM	6210 CB (6211 OG)	SER 64 SER 64 SER 64 SER 64		68 43.718 1.00 08 44.269 1.00 24 45.679 1.00		
ATOM ATOM ATOM	6213 0 6 6214 N 6 6215 CA	SER 64 ASP 65 ASP 65	124. 630 67. 4 126. 712 68. 1 127. 306 66. 9	88 44.691 1.00 76 44.236 1.00 47 44.728 1.00	31. 36 B 31. 42 B 32. 55 B	O N C
ATOM ATOM ATOM ATOM			128. 576 66. 6 129. 158 65. 2 128. 446 64. 2 130. 331 65. 2	86 44.302 1.00 61 44.158 1.00	33. 28 B 35. 12 B 33. 02 B 37. 02 B	C C O O
ATOM ATOM ATOM	6220 C / 6221 O /	ASP 65 ASP 65 HIS 66	127. 636 67. 04 128. 076 66. 06 127. 399 68. 2	45 46.211 1.00 69 46.818 1.00	32. 66 B 31. 78 B 33. 06 B	C O N

				FIG. 4-128	(Continued)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	6260 6261 6262	CA HIS CB HIS CCD HIS ND1 HIS CE1 HIS NE2 HIS C HIS O HIS NE2 HIS C HIS O GLU CA GLU CB GLU OE2 GLU OE1 GLU OE2 GLU CCB TYR CCB TYR CCB TYR CCB TYR CCB TYR CCD TYR CCB TYR CCD TYR CC	66666666666666666666666666666666666666	127. 704 68. 440 48. 203 1. 00 32. 64 128. 892 69. 402 48. 329 1. 00 35. 63 130. 032 69. 076 47. 416 1. 00 39. 09 131. 260 68. 562 47. 669 1. 00 40. 29 129. 959 69. 238 46. 047 1. 00 41. 80 131. 092 68. 835 45. 498 1. 00 42. 37 131. 897 68. 420 46. 459 1. 00 42. 11 126. 547 69. 001 49. 016 1. 00 31. 01 126. 602 69. 085 50. 245 1. 00 30. 92 125. 505 69. 479 48. 345 1. 00 30. 92 124. 379 70. 067 49. 062 1. 00 38. 07 124. 457 71. 591 48. 984 1. 00 27. 21 125. 601 72. 179 49. 781 1. 00 29. 99 125. 745 73. 675 49. 593 1. 00 32. 09 126. 408 74. 315 50. 438 1. 00 27. 52 127. 872 69. 085 <td>B C C C C C C C C C C C C C C C C C C C</td>	B C C C C C C C C C C C C C C C C C C C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	6263 6264 6265 6266 6267 6268 6269 6270 6271	CB TYR CG TYR CD1 TYR CE1 TYR CD2 TYR CE2 TYR CZ TYR OH TYR C TYR	70 70 70 70 70 70 70 70	115. 799 70. 142 53. 667 1. 00 28. 76 B 114. 910 69. 348 54. 592 1. 00 26. 47 B 114. 396 68. 114 54. 206 1. 00 25. 75 B 113. 544 67. 398 55. 038 1. 00 26. 40 B 114. 553 69. 847 55. 842 1. 00 28. 33 B 113. 701 69. 141 56. 686 1. 00 28. 03 B 113. 199 67. 918 56. 276 1. 00 28. 21 B 112. 346 67. 221 57. 103 1. 00 30. 20 B 114. 056 71. 796 52. 983 1. 00 34. 45 B	

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										(Continued)
					FIG	. 4 -	1 3 0			
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	6321 6322 6323 6324 6325 6326 6327 6328 6329 6330 6331 6332 6333 6334 6335	O N I CA I CB I CCD I CC	ILE LEU LEU LEU LEU LEU LEU LEU VAL VAL VAL	76 76 77 77 77 77 77 77 77 77 78 78 78	112. 341 115. 243 115. 758 115. 862 117. 208 117. 227 116. 155 116. 435 116. 149 118. 121 117. 657 119. 417 120. 409 121. 227 122. 327	77. 009 76. 589 77. 701 75. 472 75. 498 74. 901 75. 359 74. 728 76. 874 74. 683 73. 821 74. 967 74. 253 75. 227 74. 480	48. 967 53. 043 53. 150 53. 400 53. 941 55. 351 56. 346 57. 701 56. 460 53. 036 52. 289 53. 103 52. 308 51. 431 50. 691	1. 00 42. 01 1. 00 39. 85 1. 00 41. 15 1. 00 36. 42 1. 00 34. 28 1. 00 34. 54 1. 00 33. 23 1. 00 34. 45 1. 00 32. 91 1. 00 30. 72 1. 00 39. 87 1. 00 29. 87 1. 00 29. 01 1. 00 31. 37	B B B B B B B B B B B B B B B B B B B	C C C C C C C C C C C C C C C C C C C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	6336 6337 6338 6339 6340 6341 6342 6343 6344 6345 6346 6347 6348	CG2 C O N CA CB CG CD1 CD2 CE1 CE2	VAL VAL PHE PHE PHE PHE PHE PHE	78 78 79 79 79 79 79 79 79 79	120. 311 121. 346 121. 781 121. 660 122. 530 121. 807 120. 680 119. 499 120. 789 118. 448 119. 749 118. 573 123. 815	75. 906 73. 523 74. 087 72. 272 71. 496 70. 247 70. 531 71. 120 70. 168 71. 338 70. 382 70. 967 71. 036	50. 448 53. 263 54. 261 52. 956 53. 821 54. 338 55. 296 54. 857 56. 636 55. 733 57. 513 57. 065 53. 151	1.00 31.37 1.00 28.37 1.00 28.38 1.00 26.51 1.00 24.85 1.00 24.45 1.00 22.62 1.00 20.15 1.00 19.84 1.00 20.35 1.00 16.96 1.00 18.97 1.00 24.95	B B B B B B B B B B B B B B B B B B B	C C O N C C C C C C C C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	6349 6350 6351 6352 6353 6354 6355 6356 6359 6360 6361 6362 6363 6364 6365	O N CA CB CG OD1 ND2 C O N CA CB C	PHE ASN ASN ASN ASN ASN	79 80 80 80 80 80 80 81 81 81 81 82 82	123. 841 124. 876 126. 174 127. 276 128. 653 128. 916 129. 542 126. 156 126. 168 126. 054 126. 025 127. 167 126. 925 127. 167 129. 525 130. 820	70. 729 70. 992 70. 518 71. 307 70. 689 69. 567 71. 421 69. 077 68. 842 68. 116 66. 713 65. 819 66. 256 65. 462 66. 764 66. 351 66. 835	51. 960 53. 948 53. 517 54. 220 54. 032 54. 486 53. 364 54. 018 55. 222 53. 105 53. 496 52. 246 54. 434 55. 347 54. 222 55. 024 54. 361	1. 00 24. 94 1. 00 23. 66 1. 00 23. 32 1. 00 22. 91 1. 00 22. 91 1. 00 23. 26 1. 00 21. 99 1. 00 24. 17 1. 00 25. 80 1. 00 23. 17 1. 00 24. 07 1. 00 20. 69 1. 00 25. 23 1. 00 25. 26 1. 00 26. 73 1. 00 29. 51 1. 00 32. 02	B B B B B B B B B B B B B B B B B B B	0 N C C C O N C C C O N C C C C O C C C C
ATOM ATOM ATOM ATOM ATOM	6366 6367 6368 6369	CG CD 0E1	GLU GLU GLU GLU	82 82 82 82 82	132. 124 132. 287 132. 064 132. 659	66. 326 64. 800 64. 191 64. 209	55. 005 54. 955 53. 884 55. 995	1.00 35.72 1.00 38.90 1.00 38.71 1.00 40.81	B B B	C C O O

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										(Continued)
					FIC	G. 4-	1 3 1			(Continued)
ATOM	6370	С	GLU	82	129. 528	66. 757	56. 497	1.00 29.17	В	С
ATOM	6371	0	GLU	82	130.102	66.051	57.324	1.00 28.55	В	0
ATOM	6372	N	TYR	83	128.888	67.872	56.834	1.00 29.07	В	N
ATOM	6373	CA	TYR	83	128. 877	68.329	58. 223	1.00 28.95	В	C
ATOM	6374	CB	TYR	83	129. 504	69. 722	58. 320	1.00 30.17	В	С
ATOM	6375	CG	TYR	83	130. 821	69. 834	57. 596	1.00 33.40	В	C
ATOM	6376		TYR	83	131.914	69.049	57.963	1.00 33.79	В	Č
ATOM	6377		TYR	83	133. 120	69. 129	57. 271	1.00 36.07	В	C
ATOM	6378		TYR	83	130. 966	70. 704	56. 517	1.00 35.97	В	C
ATOM ATOM	6379 6380	CEZ	TYR TYR	83	132. 162	70. 791	55.815	1.00 36.91	В	C
ATOM	6381	OH	TYR	83 83	133. 234 134. 413	70.003 70.091	56. 195	1.00 38.12 1.00 42.42	В	C
ATOM	6382	C	TYR	83	127. 490	68. 355	55. 486 58. 853	1.00 42.42	B . B	0 C
ATOM	6383	Ö	TYR	83	127. 340	68. 093	60.044	1.00 28.10	В	0
ATOM	6384	N	GLY	84	126.478	68. 684	58. 063	1.00 25.68	В	N N
ATOM	6385	CA	GLY	84	125. 136	68. 726	58. 601	1.00 24.77	В	Č
ATOM	6386	Č	GLY	84	124.668	70. 137	58. 880	1.00 24.95	В	č
ATOM	6387	Ŏ	GLY	84	123. 511	70. 345	59. 222	1.00 23.68	В	ŏ
ATOM	6388	N	ASN	85	125.565	71.109	58.745	1.00 26.40	B	Ň
ATOM	6389	CA	ASN	85	125. 201	72.501	58.984	1.00 27.79	В	C
ATOM	6390	CB	ASN	85	126.446	73.366	59. 181	1.00 28.01	В	С
ATOM	6391	CG	ASN	85	127. 356	73. 363	57.975	1.00 31.32	В	C
ATOM	6392		ASN	85	128.051	72. 384	57. 697	1.00 31.73	В	0
ATOM	6393		ASN	85	127. 338	74. 472	57. 250	1.00 33.71	В	N
ATOM	6394	C	ASN	85	124. 381	73. 023	57.813	1.00 28.62	В	C
ATOM	6395	0	ASN	85 96	124. 432	72.472	56. 720	1.00 28.74	В	0
ATOM ATOM	6396 6397	N Ca	SER SER	86 86	123.622 122.787	74.085	58. 043	1.00 30.17	В	N
ATOM	6398	CB	SER	86 86	121. 392	74.633	56. 991	1.00 32.38	В	C
ATOM	6399	OG	SER	86	121. 392	74. 005 74. 380	57. 061 58. 256	1.00 31.71 1.00 32.32	В	C
ATOM	6400	C	SER	86	122. 658	76. 145	57. 063	1.00 32.32	B B	0
ATOM	6401	ŏ	SER	86	123. 307	76. 800	57.874	1.00 33.03	В	C 0
ATOM	6402	Ň	SER	87	121.806	76.682	56. 195	1.00 35.45	В	N N
ATOM	6403	CA	SER	87	121.530	78. 111	56. 115	1.00 35.95	В	Č
ATOM	6404	CB	SER	87	122.588	78. 825	55. 280	1.00 35.50	В	č
ATOM	6405	0G	SER	87	123.887	78.635	55.810	1.00 39.27	B	Ö
ATOM	6406	C	SER	87	120.191	78. 233	55.418	1.00 36.74	B	Č
ATOM	6407	0	SER	87	119.832	77.369	54.625	1.00 38.47	В	Ŏ
ATOM	6408		VAL	88	119.444	79. 288	55.723	1.00 37.17	В	N
ATOM	6409		VAL	88	118. 154	79.498	55. 084	1.00 36.32	В	С
ATOM	6410		VAL	88	117. 357	80.636	55. 750	1.00 37.21	В	С
ATOM	6411	CG1		88	116.094	80.916	54. 954	1.00 36.84	В	С
ATOM	6412	CG2		88	117.006	80. 260	57. 186	1.00 38.04	В	C
ATOM	6413		VAL	88	118. 422	79. 897	53. 647	1.00 36.83	В	C
ATOM	6414		VAL	88	119. 235	80. 782	53. 379	1.00 36.34	В	0
ATOM ATOM	6415 6416		PHE PHE	89 80	117.745	79. 240	52. 719	1.00 36.53	В	N
ATOM	6417		rne PHE	89 89	117. 925	79. 552	51.314	1.00 37.05	В	C
ATOM	6418		PHE	89	117. 901 118. 060	78. 262	50. 491	1.00 34.62	В	C
AT OIL	0110	ou	r III;	03	110.000	78. 474	49.014	1.00 31.67	В	С

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(Continued)
                                     FIG. 4-132
 ATOM
        6419
               CD1 PHE
                           89
                                   116.963
                                             78.790
                                                      48.223
                                                               1.00 29.04
        6420
 ATOM
               CD2 PHE
                                   119.303
                           89
                                             78.333
                                                      48.412
                                                               1.00 31.62
                                                                                       _{\rm C}^{\rm C}
 ATOM
        6421
               CE1 PHE
                           89
                                   117.095
                                             78.958
                                                      46.857
                                                               1.00 28.72
                                                                                 В
                                   119.450
 ATOM
        6422
               CE2 PHE
                                             78.500
                           89
                                                      47.038
                                                               1.00 32.27
                                                                                 В
                                                                                       C
        6423
 ATOM
               CZ
                   PHE
                                   118.342
                           89
                                             78.813
                                                      46.258
                                                               1.00 30.91
                                                                                      C
                                                                                 В
        6424
 ATOM
               C
                    PHE
                                   116.801
                           89
                                             80.483
                                                      50.896
                                                               1.00 39.38
                                                                                      Ċ
                                                                                 В
 ATOM
        6425
               0
                    PHE
                                   116.901
                           89
                                             81.188
                                                      49.892
                                                               1.00 39.89
                                                                                 В
                                                                                      0
 ATOM
        6426
               N
                    LEU
                           90
                                   115.733
                                             80.493
                                                      51.688
                                                               1.00 41.53
                                                                                 В
                                                                                      N
 ATOM
        6427
               CA
                   LEU
                           90
                                   114.581
                                             81.332
                                                      51.403
                                                               1.00 43.78
                                                                                 В
                                                                                      C
        6428
 ATOM
               CB
                   LEU
                           90
                                   113.849
                                             80.788
                                                      50.173
                                                               1.00 44.69
                                                                                 В
                                                                                      C
                                   112. 818
113. 439
 ATOM
        6429
               CG
                   LEU
                                             81.664
                           90
                                                      49.462
                                                               1.00 44.94
                                                                                 В
                                                                                      C
                   LEU
        6430
 ATOM
               CD1
                                             83.000
                           90
                                                      49.088
                                                               1.00 44.39
                                                                                 В
                                                                                      C
        6431
 ATOM
               CD2
                                   112.328
                   LEU
                           90
                                             80.944
                                                      48. 217
                                                               1.00 44.54
                                                                                 B
                                                                                      C
ATOM
        6432
               C
                   LEU
                                   113.653
                           90
                                             81.348
                                                      52.613
                                                               1.00 45.79
                                                                                 В
                                                                                      C
ATOM
        6433
               0
                   LEU
                           90
                                   113. 192
                                             80.302
                                                      53.062
                                                               1.00 44.77
                                                                                 В
                                                                                      0
ATOM
        6434
              N
                   GLU
                           91
                                   113. 395
                                             82.542
                                                      53.140
                                                               1.00 49.59
                                                                                 В
                                                                                      N
ATOM
        6435
              CA
                   GLU
                           91
                                   112.524
                                             82.715
                                                      54.302
                                                               1.00 51.78
                                                                                 В
                                                                                      \mathbb{C}
ATOM
        6436
              CB
                   GLU
                           91
                                   112.571
                                             84.166
                                                      54.790
                                                               1.00 53.90
                                                                                 В
                                                                                      C
ATOM
        6437
               CG
                   GLU
                                   113.950
                           91
                                             84.663
                                                      55.199
                                                               1.00 58.64
                                                                                В
                                                                                      C
ATOM
        6438
               CD
                   GLU
                           91
                                   114.432
                                             84.070
                                                      56.511
                                                               1.00 61.93
                                                                                В
                                                                                      C
ATOM
        6439
              0E1
                   GLU
                                   114.607
                           91
                                             82.835
                                                      56.585
                                                               1.00 64.17
                                                                                В
                                                                                      0
ATOM
        6440
              OE2 GLU
                           91
                                   114.639
                                            84.843
                                                     57.472
                                                               1.00 63.53
                                                                                В
                                                                                      0
ATOM
              C
        6441
                   GLU
                           91
                                   111.083
                                            82.352
                                                     53.961
                                                               1.00 52.17
                                                                                В
                                                                                      C
ATOM
              0
        6442
                   GLU
                           91
                                   110.549
                                            82.777
                                                     52.939
                                                              1.00 50.91
                                                                                B
                                                                                      0
ATOM
        6443
              N
                   ASN
                           92
                                   110.452
                                            81.576
                                                     54.835
                                                              1.00 53.63
                                                                                В
                                                                                      N
ATOM
        6444
              CA
                   ASN
                           92
                                   109.073
                                            81.146
                                                     54.631
                                                              1.00 54.46
                                                                                В
                                                                                      C
ATOM
        6445
              CB
                   ASN
                                   108.654
                           92
                                            80.205
                                                     55.761
                                                              1.00 55.64
                                                                                B
B
                                                                                      _{\rm C}^{\rm C}
ATOM
              CG
        6446
                   ASN
                           92
                                   108.451
                                            80.934
                                                     57.074
                                                              1.00 57.59
ATOM
        6447
              OD1 ASN
                           92
                                   109.140
                                            81.914
                                                     57.362
                                                              1.00 59.33
                                                                                В
                                                                                      0
ATOM
        6448
              ND2 ASN
                           92
                                   107.512
                                            80.451
                                                     57.885
                                                             1.00 57.67
                                                                                В
                                                                                      N
ATOM
        6449
              C
                   ASN
                           92
                                   108.116
                                            82.336
                                                     54.581
                                                              1.00 53.80
                                                                                В
                                                                                      C
ATOM
        6450
              0
                   ASN
                           92
                                   106.924
                                            82.171
                                                     54.328
                                                              1.00 53.09
                                                                                В
                                                                                      0
ATOM
                                            83.532
        6451
              N
                   SER
                           93
                                   108.646
                                                     54.818 1.00 53.62
                                                                                В
                                                                                     N
                                  107.833
ATOM
        6452
              CA
                   SER
                           93
                                            84.744
                                                     54.813 1.00 53.91
                                                                                В
                                                                                      C
ATOM
        6453
              CB
                   SER
                           93
                                  108.078
                                            85.527
                                                     56.100
                                                              1.00 53.85
                                                                                     C
ATOM
        6454
              0G
                   SER
                           93
                                  109.438
                                            85.905
                                                     56.196
                                                             1.00 54.56
                                                                                В
                                                                                     0
ATOM
       6455
              C
                   SER
                           93
                                  108.097
                                            85.658
                                                     53.618 1.00 53.82
                                                                                В
                                                                                     C
ATOM
       6456
              0
                           93
                   SER
                                  107.391
                                            86.646
                                                     53. 421
                                                              1,00 52,94
                                                                                В
                                                                                     0
ATOM
       6457
                   THR
              N
                          94
                                  109.107
                                            85.322
                                                     52.819
                                                              1.00 54.56
                                                                                В
                                                                                     N
                                            86. 127
ATOM
       6458
              CA
                   THR
                          94
                                  109.473
                                                     51.656
                                                             1.00 54.56
                                                                                В
                                                                                     C
ATOM
       6459
              CB
                   THR
                          94
                                  110.616
                                            85.473
                                                     50.858
                                                             1.00 54.40
                                                                                В
ATOM
       6460
              OG1 THR
                          94
                                  110.837
                                            86.210
                                                     49.648
                                                             1.00 53.65
                                                                                В
                                                                                     0
ATOM
       6461
              CG2 THR
                          94
                                  110.268
                                            84.040
                                                     50.515
                                                              1.00 55.54
                                                                               В
                                                                                     C
ATOM
       6462
              C
                   THR
                          94
                                  108.330
                                            86.418
                                                     50.689
                                                              1.00 54.94
                                                                                     C
                                                                               В
ATOM
       6463
              0
                   THR
                          94
                                  108.424
                                            87.339
                                                     49.878
                                                              1.00 55.42
                                                                               В
                                                                                     0
ATOM
       6464
              N
                   PHE
                          95
                                  107.256
                                            85.640
                                                     50.762
                                                              1.00 54.35
                                                                               В
                                                                                     N
ATOM
       6465
              CA
                  PHE
                          95
                                  106.125
                                            85.865
                                                     49.873
                                                             1.00 54.57
                                                                                     \begin{array}{c} C \\ C \\ C \end{array}
                                                                               В
ATOM
       6466
              CB
                  PHE
                          95
                                            84.681
                                  105.956
                                                     48.914
                                                             1.00 53.35
                                                                               В
ATOM
       6467
             CG
                  PHE
                          95
                                            84.426
                                  107.158
                                                    48.043
                                                             1.00 52.21
```

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				FIG. 4	- 1 3 3			(Continued)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	6468 6469 6470 6471 6472 6473 6474 6475 6476	CD1 PHE CD2 PHE CE1 PHE CE2 PHE CZ PHE C PHE O PHE N ASP CA ASP CB ASP	95 95 95 95 95 96 96 96	107.978 83.32 107.476 85.29 109.095 83.09 108.594 85.06 109.403 83.96 104.825 86.10 103.740 85.78 104.941 86.68 103.775 86.96 104.167 87.78 104.793 86.94	48. 268 47. 005 47. 473 46. 205 60 46. 441 55 50. 639 44 50. 149 51 51. 835 64 52. 668 85 53. 900 65 54. 993	1.00 51.86 1.00 51.89 1.00 50.37 1.00 51.43 1.00 50.62 1.00 55.66 1.00 55.16 1.00 56.69 1.00 57.24 1.00 58.96 1.00 60.91	B B B B B B B	C C C C C C O N C C C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	6479 6480 6481 6482 6483 6484 6485	OD1 ASP OD2 ASP C ASP O ASP N GLU CA GLU CB GLU CG GLU	96 96 96 97 97 97	104. 234 85. 87 105. 835 87. 36 102. 674 87. 71 101. 498 87. 40 103. 050 88. 70 102. 068 89. 49 102. 389 90. 99 102. 397 91. 55	56. 55. 538 2 51. 933 31 52. 100 33 51. 130 36 50. 395 4 50. 512 3 51. 935	1.00 60.82 1.00 62.59 1.00 57.24 1.00 58.26 1.00 57.07 1.00 57.68 1.00 59.15 1.00 61.76	B B B B B B	0 0 C 0 N C C C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	6487 6488 6489 6490 6491 6492 6493 6494	CD GLU OE1 GLU OE2 GLU C GLU O GLU N PHE CA PHE CB PHE	97 97 97 97 97 98 98	103.629 91.14 103.714 91.49 104.514 90.46 101.970 89.12 101.652 89.97 102.234 87.85 102.181 87.39 102.730 85.96	0 53. 927 7 52. 155 3 48. 917 2 48. 080 9 48. 598 3 47. 214	1.00 63.57 1.00 63.88 1.00 64.73 1.00 56.86 1.00 58.05 1.00 54.75 1.00 52.58 1.00 52.53	B B B B B	C 0 0 C 0 N C C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM	6495 6496 6497 6498 6499 6500 6501	CG PHE CD1 PHE CD2 PHE CE1 PHE CE2 PHE CZ PHE C PHE	98 98 98 98 98 98	102.792 85.43 103.564 86.07 102.064 84.30 103.609 85.59 102.103 83.82 102.876 84.46 100.764 87.44	4 45.713 44.749 5 45.348 7 43.445 2 44.044 9 43.092 8 46.641	1.00 51.74 1.00 50.75 1.00 51.54 1.00 50.51 1.00 50.40 1.00 49.83 1.00 51.24	B B B B B	C C C C C C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM	6502 6503 6504 6505 6506 6507 6508	CA GLY C GLY O GLY N HIS CA HIS	98 99 99 99 100 100	98. 383 87. 44 97. 918 86. 19 97. 020 86. 24 98. 530 85. 06 98. 200 83. 78	3 47. 523 1 47. 094 2 46. 376 6 45. 540 5 46. 712 0 46. 104	1.00 50.42 1.00 50.67 1.00 48.74 1.00 47.41 1.00 48.42 1.00 45.49 1.00 43.24	B B B B B	O N C C O N C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	6509 6510 6511 6512 6513 6514 6515 6516	CB HIS CG HIS CD2 HIS ND1 HIS CB1 HIS NE2 HIS C HIS O HIS	100 100 100 100 100 100 100	98. 787 83. 68 98. 004 84. 41 98. 345 85. 43 96. 711 84. 07 96. 288 84. 85 97. 262 85. 69 98. 822 82. 67 99. 916 82. 84	4 43. 651 7 42. 833 5 43. 321 7 42. 344 1 42. 029 7 46. 940	1.00 41.93 1.00 39.37 1.00 38.83 1.00 39.65 1.00 38.90 1.00 38.71 1.00 42.56 1.00 43.12	B B B B B	C C N C N C O

				·s.	FI	G. 4-	134			(Continued)
ATOM	6517	N	SER	101	98. 139	81.547	47. 063	1.00 41.90	В	N
ATOM	6518	CA	SER	101	98.716	80.442	47.817	1.00 43.20	В	С
ATOM	6519	CB	SER	101	97. 623		48. 382	1.00 43.41	В	С
ATOM	6520	0G	SER	101	96.852		47. 354	1.00 44.00	В	0
ATOM	6521	C	SER	101	99. 582		46.820	1.00 42.92	В	C
ATOM	6522	0	SER	101	99.083		45. 794	1.00 43.33	В	0
ATOM	6523	N	ILE	102	100.880		47.095	1.00 41.90	В	N
ATOM	6524	CA	ILE	102	101.762		46.183	1.00 42.10	. B	C
ATOM	6525	CB	ILE	102	103. 255		46.369	1.00 43.10	В	C
ATOM	6526		ILE	102	103. 370		46.404	1.00 43.52	В	C
ATOM ATOM	6527 6528	CD1	ILE ILE	102 102	103.824		47.660	1.00 45.01	В	C
ATOM	6529	CDI	ILE	102	105. 294 101. 598		47.895 46.415	1.00 46.96 1.00 41.08	В	C C
ATOM	6530	Õ	ILE	102	101. 538		47. 544	1.00 41.08	B B	0
ATOM	6531	N	ASN	102	101.342		45. 339	1.00 41.27	В	N
ATOM	6532	CA	ASN	103	101. 157		45. 434	1.00 40.03	В	C
ATOM	6533	CB	ASN	103	100.502		44. 163	1.00 39.98	В	Č
ATOM	6534	CG	ASN	103	100.190		44. 257	1.00 39.82	В	Č
ATOM	6535		ASN	103	99. 355		45. 056	1.00 40.83	В	ŏ
ATOM	6536		ASN	103	100.866		43. 448	1.00 40.75	. B	Ň
ATOM	6537	C	ASN	103	102.486	74.508	45.645	1.00 37.42	B	Ċ
ATOM	6538	0	ASN	103	102.601	73.614	46.475	1.00 38.46	B	Ö
ATOM	6539	N	ASP	104	103.491	74.912	44.880	1.00 35.77	В	Ň
ATOM	6540	CA	ASP	104	104.808	74.303	44.982	1.00 34.14	В	C
ATOM	6541	CB	ASP	104	104.819	72.955	44. 248	1.00 33.54	В	C
ATOM	6542	CG	ASP	104	105.987	72.072	44.655	1.00 34.77	В	C
ATOM	6543	OD1		104	106.061	70.919	44.178	1.00 33.72	В	0
ATOM	6544	OD2		104	106. 835	72. 525	45. 453	1.00 35.84	В	0
ATOM	6545	C	ASP	104	105. 827	75. 253	44. 367	1.00 33.07	В	C
ATOM	6546	0	ASP	104	105. 461	76. 218	43.695	1.00 33.54	В	0
ATOM	6547	N	TYR	105	107. 103	74. 985	44.607	1.00 32.32	В	N
ATOM	6548	CA	TYR	105	108. 167	75.824	44.082	1.00 31.45	В	C
ATOM	6549	CB	TYR	105	108. 854	76. 573	45. 220	1.00 32.58	В	C
ATOM ATOM	6550 6551	CG CD1	TYR	105	109.515	75. 662	46. 218	1.00 35.82	В	C
ATOM	6552	CE1		105 105	110.859	75.306	46.091	1.00 36.01	В	C
ATOM	6553	CD2		105	111. 465 108. 791	74. 453 75. 138	47. 287	1.00 36.30	В	C
ATOM	6554	CE2		105	109. 387	74. 282	48. 208	1.00 37.55 1.00 38.47	В	C
ATOM	6555	CZ	TYR	105	110.719	73. 947	48. 065	1.00 36.47	B B	C
ATOM	6556	OH	TYR	105	111. 293	73. 106	48. 984	1.00 38.67	В	C
ATOM	6557	C	TYR	105	109. 180	74. 972	43. 347	1.00 30.07	В	0 C
ATOM	6558		TYR	105	109.048	73. 754	43. 276	1.00 29.32	В	Õ
ATOM	6559	Ň	SER	106	110. 203	75. 623	42.815	1.00 28.45	В	N
ATOM	6560		SER	106	111. 236	74. 938	42.059	1.00 26.63	В	C
ATOM	6561		SER	106	110.648	74. 391	40. 758	1.00 24.49	B	Č
ATOM	6562		SER	106	111.662	74. 145	39.806	1.00 24.16	B	ŏ
ATOM	6563		SER	106	112. 341	75. 926	41.745	1.00 26.32	В	č
ATOM	6564		SER	106	112. 168	76. 821	40.919	1.00 28.04	\tilde{B}	ŏ
ATOM	6565	N	ILE	107	113.475	75.770	42.413	1.00 25.01	В	N

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										(Continued)
					FIC	S. 4 -	136			Continued
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	6615 6616 6617 6618 6619 6620 6621 6622 6623 6624 6625 6626	CG1	PHE PHE PHE ILE ILE ILE ILE ILE ILE	113 113 114 114 114 114 114 114 114 114	FIC 117. 386 114. 831 115. 308 113. 557 112. 630 112. 394 111. 911 111. 378 111. 336 111. 336 110. 895 110. 756	85. 152 80. 896 79. 829 81. 205 80. 258 80. 504 81. 915 79. 490 79. 367 80. 403 81. 508 79. 265	36. 819 41. 058 41. 425 41. 219 41. 791 43. 293 43. 529 43. 813 45. 325 41. 019 40. 715 40. 671	1. 00 35. 71 1. 00 30. 65 1. 00 30. 90 1. 00 30. 09 1. 00 29. 81 1. 00 28. 60 1. 00 29. 81 1. 00 30. 57 1. 00 33. 23 1. 00 29. 79 1. 00 28. 83 1. 00 30. 43	B B B B B B B B B B B B B B B B B B B	C C O N C C C C C C
ATOM ATOM ATOM	6627 6628 6629	CA CB CG	LEU LEU LEU	115 115 115	109. 516 109. 596 108. 449	79. 223 78. 108 77. 898	39. 925 38. 890 37. 912	1. 00 29. 05 1. 00 28. 31 1. 00 28. 22	B B B	C C C
ATOM ATOM ATOM ATOM	6630 6631 6632 6633	CD2 C 0	LEU LEU LEU LEU	115 115 115 115	108. 425 108. 645 108. 424 108. 370	79. 001 76. 553 78. 923 77. 824	36. 872 37. 245 40. 932 41. 483	1.00 28.47 1.00 29.52 1.00 29.59 1.00 30.72	B B B	C C C O
ATOM ATOM ATOM ATOM	6634 6635 6636 6637		LEU LEU LEU LEU	116 116 116 116	107. 568 106. 479 106. 129 107. 277	79. 901 79. 699 81. 001 81. 741	41. 196 42. 142 42. 861 43. 544	1.00 30.29 1.00 30.17 1.00 31.28 1.00 33.66	В В В В	N C C C
ATOM ATOM ATOM ATOM	6638 6639 6640 6641	CD1 CD2 C		116 116 116 116	106. 732 107. 957 105. 270 104. 835	82. 988 80. 821 79. 215 79. 845	44. 229 44. 552 41. 369 40. 401	1. 00 33. 41 1. 00 34. 07 1. 00 30. 44 1. 00 30. 69	В В В В	C C C O
ATOM ATOM ATOM ATOM	6642 6643 6644 6645	N CA CB CG	GLU GLU GLU GLU	117 117 117 117	104. 724 103. 563 103. 813 102. 671	78. 091 77. 513 76. 017 75. 210	41. 804 41. 159 40. 963 40. 368	1. 00 30. 37 1. 00 29. 50 1. 00 30. 63 1. 00 32. 07	B B B	N C C C
ATOM ATOM ATOM ATOM	6646 6647 6648 6649	CD OE1 OE2 C	GLU GLU	117 117 117 117	103. 023 103. 772 102. 566 102. 312	73. 728 73. 341 72. 956 77. 756	40. 270 39. 340 41. 140 42. 009	1.00 33.58 1.00 32.53 1.00 32.35 1.00 29.67	B B B	C 0 0 C
ATOM ATOM ATOM ATOM	6650 6651 6652 6653	O N CA CB	GLU TYR TYR TYR	117 118 118 118	102. 333 101. 235 99. 966 99. 928		43. 228 41. 355 42. 026 42. 643	1. 00 27. 89 1. 00 29. 27 1. 00 28. 00 1. 00 29. 37	B B B	O N
ATOM ATOM ATOM ATOM	6654 6655 6656 6657	CG CD1 CE1	TYR TYR TYR TYR	118 118 118 118	100. 036 101. 256 101. 355 98. 915	80. 955 81. 301 82. 373 81. 703	41. 659 41. 092 40. 210 41. 316	1.00 29.69 1.00 30.04 1.00 31.36 1.00 30.41	B B B	C C C C C
ATOM ATOM ATOM ATOM	6658 6659 6660 6661		TYR TYR TYR TYR	118 118 118 118	99. 003 100. 222 100. 298 98. 814	82. 768 83. 101 84. 179 78. 240	40. 439 39. 891 39. 039 41. 038	1.00 31.17 1.00 31.56 1.00 33.43 1.00 27.66	B B B	C C O C
ATOM ATOM	6662 6663	0 N	TYR ASN	118 119	99. 046 97. 582	77. 917 78. 450	39. 874 41. 499	1.00 26.73 1.00 27.22	B B	O N

										(Continued)
					FIG.	4 -	1 3 7			(Continued)
ATOM	6664	CA	ASN	119	96. 397 78	. 261	40.659	1.00 27.10	В	С
ATOM	6665	CB	ASN	119		. 203	39. 449	1.00 27.22	B	č
ATOM	6666	ČĞ	ASN	119		. 599	39.777	1.00 27.62	В	С
ATOM	6667	0D1		119		. 761	40.456	1.00 26.76	В	0
ATOM	6668	ND2		119		.612	39. 277	1.00 25.87	В	N
ATOM	6669	C	ASN	119		. 810	40.171	1.00 27.88	В	С
ATOM	6670	0	ASN	119		. 534	39.045	1.00 27.93	В	0
ATOM	6671	N	TYR	120		. 888	41.028	1.00 27.57	В	N
ATOM	6672	CA	TYR	120		. 466	40.702	1.00 29.01	В	C
ATOM	6673	CB	TYR	120		. 669	41.866	1.00 30.85	В	C
ATOM	6674	CG	TYR	120		. 171	41.635	1.00 32.83	В	C
ATOM	6675	CD1		120		. 568	40.940	1.00 33.76	В	C
ATOM	6676	CE1		120		. 190	40.717	1.00 35.03	В	C
ATOM	6677	CD2		120		. 358	42.100	1.00 34.41	В	C
ATOM ATOM	6678 6679	CE2 CZ	TYR TYR	120 120		. 981 . 403	41.880 41.191	1.00 34.35 1.00 35.47	B B	C C
ATOM	6680	OH	TYR	120		. 039	40. 987	1.00 35.47	В	0
ATOM	6681	C	TYR	120		. 863	40. 364	1.00 33.30	В	Č
ATOM	6682	Ö	TYR	120		. 034	41.099	1.00 23.11	В	0 .
ATOM	6683	Ň	VAL	121		. 148	39. 248	1.00 27.53	В	N .
ATOM	6684	ĊA	VAL	121		. 487	38. 842	1.00 25.45	В	Č
ATOM	6685	CB	VAL	121		. 296	37. 785	1.00 25.23	B	č
ATOM	6686	CG1		121		. 534	37. 376	1.00 22.18	B	Č
ATOM	6687	CG2	VAL	121		. 666	38.354	1.00 21.81	В	Ċ
ATOM	6688	C	VAL	121	94.527 71	. 130	38. 275	1.00 24.99	В	C
ATOM	6689		VAL	121		. 031	37. 242	1.00 24.18	В	0
ATOM	6690		LYS	122		. 082	38. 977	1.00 24.16	В	N
ATOM	6691		LYS	122		. 735	38. 570	1.00 24.24	В	C
ATOM	6692		LYS	122	94. 295 67	. 780	39. 754	1.00 23.05	В	C
ATOM	6693		LYS	122		. 327	39. 390	1.00 20.04	В	C
ATOM	6694		LYS	122		. 416	40. 589	1.00 20.19	В	C
ATOM	6695		LYS	122		. 950	40. 161	1.00 20.85	В	Ç
ATOM ATOM	6696 6697		LYS	122		. 632	39. 136	1.00 18.96	В	N
ATOM	6698		LYS LYS	122 122		. 180	37. 387	1.00 24.10	В	C
ATOM	6699		GLN	123		. 488 . 368	37. 189	1.00 23.23	В	0
ATOM	6700		GLN	123		. 691	36. 592 35. 472	1.00 23.36 1.00 21.22	В	N C
ATOM	6701		GLN	123		. 007	34. 145	1.00 20.62	B B	C C
ATOM	6702		GLN	123		433	32. 948	1.00 20.02	В	C
ATOM	6703		GLN	123		857	31. 591	1.00 24.37	В	Č
ATOM	6704		GLN	123		606	31. 275	1.00 26.71	В	0
ATOM	6705	NE2		123		493	30. 779	1.00 23.80	B	Ň
ATOM	6706	C	GLN	123		194	35. 805	1.00 20.06	B	Ċ
ATOM	6707		GLN	123		741	36. 786	1.00 17.04	B	Ŏ
ATOM	6708		TRP	124		438	35.030	1.00 17.49	B	Ň
ATOM	6709		TRP	124	94. 753 63.	009	35. 276	1.00 16.75	В	Č
ATOM	6710		TRP	124		298	33.984	1.00 16.19	В	С
ATOM	6711		TRP	124			32. 797	1.00 18.11	В	С
ATOM	6712	CD2	IKL	124			32. 764	1.00 17.55	В	С
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ATOM 6713 CE2 TRP 124 92.630 63.449 31.455 1.00 16.84 B C ATOM 6714 CE3 TRP 124 91.909 62.942 33.713 1.00 17.02 B C ATOM 6715 CD1 TRP 124 94.819 62.999 31.539 1.00 19.00 B C ATOM 6716 NB1 TRP 124 91.331 63.815 13.067 1.00 15.16 B C ATOM 6716 NB1 TRP 124 91.331 63.815 13.067 1.00 15.16 B C ATOM 6718 C22 TRP 124 91.331 63.815 31.067 1.00 15.16 B C ATOM 6718 C22 TRP 124 90.342 63.737 32.011 1.00 16.12 B C ATOM 6719 CH2 TRP 124 95.816 63.305 33.326 1.00 16.85 B C ATOM 6719 CH2 TRP 124 95.816 63.437 37.320 11 1.00 17.28 B C ATOM 6720 C TRP 124 95.816 63.437 37.397 1.00 17.74 B O ATOM 6721 O TRP 124 95.816 63.437 37.397 1.00 17.74 B O ATOM 6722 N ARG 125 96.430 61.560 63.391 1.00 16.12 B C ATOM 6723 CA ARG 125 97.317 61.185 37.429 1.00 16.66 B C ATOM 6723 CA ARG 125 97.666 59.702 37.323 1.00 16.96 B C ATOM 6726 CD ARG 125 98.689 57.987 38.794 1.00 18.35 B C ATOM 6726 CD ARG 125 98.08 59.288 38.076 1.00 18.35 B C ATOM 6726 CD ARG 125 98.689 57.987 38.794 1.00 18.85 B C ATOM 6727 NE ARG 125 98.698 59.288 38.076 1.00 18.35 B C ATOM 6720 NH2 ARG 125 97.666 59.702 37.323 1.00 16.96 B C ATOM 6720 NH2 ARG 125 99.698 59.288 38.076 1.00 18.85 B C ATOM 6720 NH2 ARG 125 99.698 59.283 38.076 1.00 18.85 B C ATOM 6720 NH2 ARG 125 99.698 59.283 38.076 1.00 18.85 B C ATOM 6731 C ARG 125 99.075 62.227 38.674 1.00 17.58 B C ATOM 6732 CD ARG 125 99.075 62.227 37.568 1.00 18.57 B N ATOM 6731 C ARG 125 99.075 62.227 37.568 1.00 18.87 B N ATOM 6731 C ARG 125 99.075 62.227 38.674 1.00 18.86 B O ATOM 6736 CG HIS 126 101.391 62.631 39.776 1.00 17.03 B N ATOM 6736 CG HIS 126 101.391 62.631 39.776 1.00 17.75 B N ATOM 6736 CG HIS 126 101.599 60.084 35.581 1.00 18.87 B C ATOM 6736 CG HIS 126 101.591 60.084 35.581 1.00 18.87 B C ATOM 6736 CG HIS 126 101.591 60.084 35.581 1.00 18.87 B C ATOM 6736 CG HIS 126 101.591 60.084 35.581 1.00 18.89 B C ATOM 6736 CG HIS 126 101.591 60.084 35.581 1.00 18.89 B C ATOM 6736 CG HIS 126 101.591 60.084 35.581 1.00 18.89 B C ATOM 6736 CG HIS 126 101.591 60.084 35.581 1.00 18.89 B C ATOM 6736 CG HIS 126 101.591 60.0											(Continued)
ATOM 6714 CB3 TRP 124 91.909 62.942 33.713 1.00 17.02 B C ATOM 6715 CD1 TRP 124 94.819 62.999 31.539 1.00 19.00 B C ATOM 6716 NB1 TRP 124 99.3794 63.429 30.731 1.00 18.26 B N ATOM 6717 CZ2 TRP 124 90.3794 63.429 30.731 1.00 18.26 B N ATOM 6718 CZ3 TRP 124 90.3794 63.429 30.731 1.00 18.26 B C ATOM 6719 CH2 TRP 124 90.342 63.737 32.011 1.00 16.12 B C ATOM 6720 C TRP 124 90.342 63.737 32.011 1.00 16.12 B C ATOM 6721 O TRP 124 95.816 63.437 37.397 1.00 17.74 B O ATOM 6722 N ARG 125 96.430 61.560 36.339 1.00 15.31 B N ATOM 6723 CA ARC 125 96.430 61.560 36.339 1.00 15.31 B N ATOM 6724 CB ARG 125 97.666 97.002 37.323 1.00 16.96 B C ATOM 6725 CC ARG 125 98.908 59.288 38.076 1.00 18.35 B C ATOM 6726 CD ARG 125 98.608 57.987 33.791 1.00 17.58 B C ATOM 6727 NE ARG 125 98.608 57.987 38.794 1.00 18.35 B C ATOM 6728 CZ ARG 125 98.608 57.987 38.794 1.00 18.57 B N ATOM 6728 CZ ARG 125 97.547 55.842 38.475 1.00 17.58 B C ATOM 6730 NH2 ARG 125 97.626 99.494 37.633 1.00 18.57 B N ATOM 6730 NH2 ARG 125 97.626 99.75 34.944 37.633 1.00 18.56 B N ATOM 6730 NH2 ARG 125 99.697 55.621 39.776 1.00 17.03 B N ATOM 6731 C ARG 125 98.698 57.987 38.794 1.00 18.57 B N ATOM 6732 CA ARG 125 99.099 62.533 36.454 1.00 18.50 B N ATOM 6733 NH 13 126 99.099 62.533 36.454 1.00 18.50 B N ATOM 6735 CB HIS 126 101.391 62.673 35.673 1.00 18.72 B C ATOM 6736 CG HIS 126 101.721 61.295 36.151 1.00 17.03 B N ATOM 6737 CD2 HIS 126 101.721 61.295 36.151 1.00 17.75 B C ATOM 6738 CB HIS 126 101.721 61.295 36.151 1.00 19.88 B C ATOM 6737 CD2 HIS 126 101.721 61.295 36.151 1.00 18.20 B C ATOM 6738 CB HIS 126 100.300 63.353 36.454 1.00 18.20 B C ATOM 6736 CB HIS 126 100.300 63.353 36.447 1.00 18.20 B C ATOM 6737 CD2 HIS 126 100.300 63.353 36.437 1.00 18.72 B C ATOM 6738 CB HIS 126 100.300 63.353 36.437 1.00 18.72 B C ATOM 6736 CB HIS 126 100.300 63.353 36.437 1.00 18.72 B C ATOM 6737 CD2 HIS 126 100.300 63.353 37.512 1.00 19.55 B C ATOM 6737 CD2 HIS 126 100.300 63.35 33 1.00 10.00 17.75 B C ATOM 6740 CB HS 126 100.300 63.35 33 1.00 10.00 17.75 B C ATOM 6740 CB HS 127						FIC	. 4 -	1 3 8			
ATOM 6714 CE3 TRP 124 91.909 62.942 33.713 1.00 17.02 B C ATOM 6715 CD1 TRP 124 94.819 62.999 31.539 1.00 19.00 B C ATOM 6716 NE1 TRP 124 99.3794 63.429 30.731 1.00 18.26 B N ATOM 6717 CZ2 TRP 124 90.3794 63.429 30.731 1.00 18.26 B N ATOM 6718 CZ3 TRP 124 90.316 63.815 31.067 1.00 15.16 B C ATOM 6719 CH2 TRP 124 90.342 63.737 32.011 1.00 16.85 B C ATOM 6720 C TRP 124 90.342 63.737 32.011 1.00 16.12 B C ATOM 6721 O TRP 124 95.816 63.437 37.397 1.00 17.28 B C ATOM 6722 N ARG 125 96.430 61.560 36.339 1.00 15.31 B N ATOM 6723 CA ARC 125 97.317 61.185 37.429 1.00 16.96 B C ATOM 6726 CD ARG 125 98.689 57.927 37.323 1.00 16.96 B C ATOM 6727 C BARC 125 98.689 57.02 37.323 1.00 16.96 B C ATOM 6727 NE ARG 125 98.689 57.927 37.323 1.00 18.35 B C ATOM 6728 CZ ARG 125 98.689 57.937 37.91 1.00 18.57 B N ATOM 6728 CZ ARG 125 98.693 55.828 38.076 1.00 18.57 B N ATOM 6728 CZ ARG 125 98.694 56.965 37.972 1.00 18.57 B N ATOM 6728 CZ ARG 125 98.694 56.945 34.94 37.633 1.00 18.57 B N ATOM 6730 NH2 ARG 125 97.567 55.621 39.776 1.00 17.58 B C ATOM 6730 NH2 ARG 125 99.694 36.944 37.693 1.00 18.57 B N ATOM 6730 NH2 ARG 125 99.695 55.621 39.776 1.00 17.03 B N ATOM 6731 C ARG 125 99.099 62.533 36.454 1.00 18.50 B C ATOM 6732 C ARG 125 99.099 62.533 36.454 1.00 18.50 B N ATOM 6733 N HIS 126 100.300 63.353 36.487 1.00 18.50 B C ATOM 6735 CB HIS 126 101.391 62.673 35.6151 1.00 19.88 B C ATOM 6737 CD2 HIS 126 101.721 61.295 36.151 1.00 19.88 B C ATOM 6738 CB HIS 126 101.391 62.673 35.6131 1.00 18.20 B C ATOM 6737 CD2 HIS 126 101.791 61.295 36.151 1.00 19.88 B C ATOM 6738 CB HIS 126 100.300 63.353 36.487 1.00 18.20 B C ATOM 6736 CB HIS 126 100.300 63.353 36.487 1.00 18.72 B C ATOM 6737 CD2 HIS 126 100.799 64.772 35.661 1.00 17.75 B N ATOM 6738 CB HIS 126 100.301 63.35 37.512 1.00 18.20 B C ATOM 6738 CB HIS 126 100.301 63.35 37.512 1.00 18.70 B C ATOM 6737 CD2 HIS 126 100.301 63.35 37.512 1.00 16.75 B C ATOM 6736 CB HIS 126 100.301 63.63 37.512 1.00 16.75 B C ATOM 6744 CA SER 127 98.909 65.309 37.301 1.00 17.75 B C ATOM 6746 CB SER 127 98.909	ATOM	6713	CE2	TRP	124	92, 630	63. 449	31.455	1.00 16.84	В	С
ATOM 6715 CD1 TRP 124 93.819 62.999 31.539 1.00 19.00 B C ATOM 6716 NB1 TRP 124 93.794 63.429 30.731 1.00 18.26 B N ATOM 6717 C22 TRP 124 90.615 63.305 33.736 1.00 16.15 B C ATOM 6719 CH2 TRP 124 90.615 63.305 33.326 1.00 16.85 B C ATOM 6719 CH2 TRP 124 90.615 63.305 33.326 1.00 16.12 B C ATOM 6720 C TRP 124 95.718 62.679 36.427 1.00 17.28 B C ATOM 6721 O TRP 124 95.718 62.679 36.427 1.00 17.28 B C ATOM 6722 N ARC 125 96.430 61.660 36.393 1.00 15.31 B N ATOM 6723 CA ARG 125 97.317 61.185 37.429 1.00 17.74 B O ATOM 6725 CC ARC 125 98.689 57.092 37.323 1.00 16.66 B C ATOM 6726 CD ARG 125 98.689 57.987 38.794 1.00 18.35 B C ATOM 6728 N ARC 125 98.689 57.987 38.794 1.00 18.35 B C ATOM 6729 NH1 ARG 125 96.972 54.944 37.693 1.00 18.57 B N ATOM 6730 NH2 ARC 125 96.972 54.944 37.693 1.00 16.56 B C ATOM 6731 C ARC 125 96.972 55.842 38.475 1.00 17.58 B C ATOM 6732 C ARC 125 96.972 54.944 37.693 1.00 18.57 B N ATOM 6733 C ARC 125 96.972 54.944 37.693 1.00 18.56 B C ATOM 6734 C B RC 125 99.695 37.987 38.794 1.00 18.57 B N ATOM 6735 C B HIS 126 100.300 63.353 36.457 1.00 18.56 B N ATOM 6736 C B HIS 126 101.391 62.673 35.641 1.00 18.06 B N ATOM 6737 NB ARC 125 99.697 547 55.621 39.776 1.00 18.50 B N ATOM 6738 N HIS 126 100.300 63.353 36.457 1.00 18.50 B N ATOM 6738 N HIS 126 101.391 60.673 35.613 1.00 18.06 B C ATOM 6737 CB HIS 126 101.391 60.673 35.613 1.00 18.20 B C ATOM 6738 ND HIS 126 101.391 60.673 35.613 1.00 18.20 B C ATOM 6738 ND HIS 126 101.591 60.084 35.581 1.00 18.20 B C ATOM 6740 RE HIS 126 100.099 62.533 36.457 1.00 18.20 B C ATOM 6740 RE HIS 126 100.099 62.533 36.457 1.00 18.20 B C ATOM 6737 CD2 HIS 126 101.391 60.673 35.611 1.00 19.88 B C ATOM 6740 RE HIS 126 100.099 62.533 36.457 1.00 18.20 B C ATOM 6740 RE HIS 126 100.099 62.533 36.457 1.00 18.20 B C ATOM 6756 C C TR 128 99.975 65.349 37.597 1.00 16.08 B N ATOM 6756 C C TR 128 99.975 65.349 37.379 1.00 17.70 B C ATOM 6756 C C TR 128 99.975 65.349 37.379 1.00 17.80 B C ATOM 6757 C TR 128 99.975 67.547 55.35 65.10 1.00 17.70 B C ATOM 6756 C C TR 128 99.975 60.									1.00 17.02	В	C
ATOM 6717 CZ2 TRP 124 91.331 63.815 31.067 1.00 15.16 B C ATOM 6718 CZ3 TRP 124 90.615 63.305 33.326 1.00 16.12 B C ATOM 6719 CH2 TRP 124 90.615 63.305 33.326 1.00 16.12 B C ATOM 6720 C TRP 124 95.718 62.679 36.427 1.00 17.28 B C ATOM 6721 O TRP 124 95.718 62.679 36.427 1.00 17.28 B C ATOM 6722 N ARC 125 96.430 61.560 36.339 1.00 15.31 B N ATOM 6723 CA ARC 125 97.317 61.185 37.429 1.00 16.66 B C ATOM 6723 CA ARC 125 97.317 61.185 37.429 1.00 16.66 B C ATOM 6724 CB ARG 125 97.666 59.702 37.323 1.00 16.96 B C ATOM 6725 CC ARC 125 98.908 59.288 38.076 1.00 18.35 B C ATOM 6726 CD ARC 125 98.689 57.987 38.794 1.00 18.57 B N ATOM 6727 NE ARG 125 97.547 55.842 38.475 1.00 17.58 B C ATOM 6728 CZ ARC 125 97.547 55.842 38.475 1.00 17.58 B C ATOM 6730 NH2 ARC 125 97.626 55.621 39.7676 1.00 18.57 B N ATOM 6730 NH2 ARC 125 98.582 62.027 37.568 1.00 18.57 B N ATOM 6731 C ARC 125 98.582 62.027 37.568 1.00 18.56 B C ATOM 6733 N H13 RC 125 98.582 62.027 37.568 1.00 18.54 B C ATOM 6733 CD ARC 125 98.582 62.027 37.568 1.00 18.54 B C ATOM 6734 CA HIS 126 100.300 63.353 36.487 1.00 17.03 B N ATOM 6735 CB HIS 126 101.319 62.673 35.644 1.00 18.06 B C ATOM 6737 CD HIS 126 101.319 62.673 35.644 1.00 18.20 B C ATOM 6737 CD HIS 126 101.319 62.673 35.644 1.00 18.06 B C ATOM 6737 CD HIS 126 101.319 62.673 35.644 1.00 18.06 B C ATOM 6737 CD HIS 126 101.319 62.673 35.644 1.00 18.06 B C ATOM 6736 CG HIS 126 101.319 62.673 35.644 1.00 18.06 B C ATOM 6737 CD HIS 126 100.300 63.353 36.487 1.00 18.72 B C ATOM 6740 NE2 HIS 126 100.301 63.353 36.487 1.00 18.75 B N ATOM 6740 NE2 HIS 126 100.303 63.353 36.487 1.00 18.70 B C ATOM 6740 NE2 HIS 126 100.304 63.353 35.611 1.00 18.72 B C ATOM 6740 NE2 HIS 126 100.305 63.353 36.487 1.00 18.78 B C ATOM 6740 NE2 HIS 126 100.307 63.355 11.00 18.79 B C ATOM 6740 NE2 HIS 126 100.307 63.355 11.00 18.79 B C ATOM 6740 NE2 HIS 126 100.307 63.355 11.00 17.70 B C ATOM 6740 NE2 HIS 126 100.307 63.355 11.00 17.70 B C ATOM 6740 NE2 HIS 126 100.307 63.355 11.00 17.70 B C ATOM 6755 CD TYR 128 99.975 71.00 60.60 40.70 17.70			CD1	TRP	124	94.819	62.999				
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TILON OTT TILL THE TOURING TOUR OFFICE THAT MAKES IN C.	ATOM	6758	OH	TYR	128	103. 190	70. 572	38. 603	1.00 20.16	$\tilde{\mathtt{B}}$	Ö
ATOM 6759 C TYR 128 97.977 70.897 34.992 1.00 19.77 B C											
ATOM 6760 O TYR 128 98.970 70.972 34.268 1.00 21.70 B O		6760			128			34. 268	1.00 21.70	В	0
ATOM 6761 N THR 129 97.239 71.955 35.291 1.00 20.48 B N	ATOM	6761	N	THR	129		71.955	35. 291	1.00 20.48	В	N

								(Continued)
			FIG	. 4 -	1 3 9			,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,
ATOM 67	763 CB 764 OG1 765 CG2 766 C 767 O 768 N 769 CA 770 CB 771 C 772 O 773 N 774 CA 775 CB 776 OG 777 C 778 O 777 C 778 CB 777 C 778 CB 777 C 778 CB 777 C 778 CB 777 C 778 CB 777 CC 778 CB 778 CB 777 CC 778 CB 777 CC 778 CB 778 CB	THR 129 THR 129 THR 129 ALA 130 ALA 130 ALA 130 ALA 130 ALA 130 SER 131 SER 131 SER 131 SER 131 SER 131 TYR 132	97. 647 96. 599 95. 353 96. 428 97. 856 97. 462 98. 474 98. 754 99. 789 99. 269 99. 514 99. 934 99. 056 97. 713 101. 290 101. 448 102. 272 103. 611 104. 179 103. 082 102. 696 104. 887 104. 510 103. 415 103. 023	73. 276 73. 968 74. 045 73. 213 74. 136 73. 765 75. 289 76. 222 75. 631 77. 525 77. 632 78. 523 79. 818 80. 948 80. 775 79. 851 79. 334 80. 438 80. 506 79. 634 77. 721 76. 383 77. 250 75. 911 75. 486 74. 171	34. 840 33. 950 34. 652 32. 634 36. 069 37. 182 35. 854 36. 926 37. 859 36. 338 35. 133 37. 199 36. 796 37. 333 36. 913 37. 463 38. 569 36. 792 37. 347 36. 516 35. 791 35. 834 37. 283 37. 283 37. 332 36. 609 36. 677	1. 00 22. 26 1. 00 23. 04 1. 00 24. 93 1. 00 22. 70 1. 00 22. 23 1. 00 20. 98 1. 00 22. 77 1. 00 23. 41 1. 00 19. 73 1. 00 26. 66 1. 00 27. 20 1. 00 29. 67 1. 00 30. 14 1. 00 30. 56 1. 00 32. 67 1. 00 32. 67 1. 00 30. 79 1. 00 30. 79 1. 00 30. 79 1. 00 32. 02 1. 00 31. 40 1. 00 26. 45 1. 00 26. 58 1. 00 26. 58 1. 00 25. 59 1. 00 25. 63	B B B B B B B B B B B B B B B B B B B	Continued) C C C C C C C C C C C C C C C C C C
ATOM 67 ATOM 67 ATOM 67 ATOM 67 ATOM 67	787 CZ 788 OH 789 C 790 O 791 N 792 CA 793 CB 794 CG 795 OD1 796 OD2 797 C 798 O 799 N 799 N 799 OCA 790 CA 790 CA	TYR 132 TYR 132 TYR 132 TYR 133 ASP 133 ASP 133 ASP 133 ASP 133 ASP 133 ASP 133 ILE 134 ILE 134 ILE 134 ILE 134 ILE 134 ILE 134	103. 415 103. 023 104. 143 103. 743 105. 041 105. 674 104. 954 103. 732 102. 805 103. 702 107. 112 107. 385 108. 031 109. 444 110. 267 111. 718 109. 649 110. 204	75. 486 74. 171 81. 929 82. 790 82. 165 83. 465 84. 287 85. 008 84. 332 86. 253 83. 228 82. 438 83. 764 83. 750 83. 392 82. 737 82. 794	36.609	1.00 25.59	В	C
ATOM 68 ATOM 68 ATOM 68 ATOM 68 ATOM 68	06 0 07 N 1 08 CA 1 09 CB 1	ILE 134 ILE 134 TYR 135 TYR 135 TYR 135 TYR 135	109. 521 110. 662 111. 167 110. 657	86. 065 84. 573 85. 539 85. 174	39. 261 40. 507 41. 475 42. 868	1.00 34.02 1.00 33.25 1.00 35.09 1.00 36.09 1.00 36.66	B B B B	C O N C C

		FIG. 4-140	(Continued)
ATOM 6812 ATOM 6813 ATOM 6814 ATOM 6815 ATOM 6816 ATOM 6816 ATOM 6817 ATOM 6817 ATOM 6818 ATOM 6821 ATOM 6821 ATOM 6822 ATOM 6823 ATOM 6824 ATOM 6825 ATOM 6826 ATOM 6827 ATOM 6828 ATOM 6828 ATOM 6830 ATOM 6831 ATOM 6833 ATOM 6834 ATOM 6836 ATOM 6837 ATOM 6838 ATOM 6837 ATOM 6838 ATOM 6838 ATOM 6840 ATOM 6841 ATOM 6841 ATOM 6842 ATOM 6843 ATOM 6844 ATOM 6844 ATOM 6845 ATOM 6845 ATOM 6845 ATOM 6850 ATOM 6851 ATOM 6853	CE1 TYR 13 CD2 TYR 13 CE2 TYR 13 CE2 TYR 13 OH TYR 13 C TYR 13 O TYR 13 N ASP 13 CA ASP 13 CG ASP 13 OD1 ASP 13 OD2 ASP 13 OD2 ASP 13 CG ASP 13 CG ASP 13 CG LEU 13 CCB LEU 13 CCB LEU 14 CCB LEU 14 CCB LEU 14 CCB LEU 15 CCB LEU 16 CCB LEU 17 CCB LEU 17 CCB LEU 17 CCB LEU 18 CCB ASN 18 C	FIG. 4 - 140 15. 110.635 87.222 44.363 1.00 34.73 B 111.134 87.971 45.424 1.00 34.55 B 112.332 85.573 44.729 1.00 35.12 B 112.839 86.316 45.786 1.00 35.07 B 112.235 87.515 46.131 1.00 35.31 B 112.740 88.258 47.179 1.00 35.05 B 112.688 85.511 41.470 1.00 38.19 B 113.293 84.517 41.873 1.00 37.81 B 113.304 86.600 41.014 1.00 40.56 B 114.759 86.692 40.965 1.00 42.09 B 15.187 87.969 40.237 1.00 42.45 B 16.690 88.051 40.030 1.00 43.61 B 17.107 88.577 38.978 1.00 45.53 B 114.972 87.522 43.209 1.00 44.492 B 116.761 85.577 43.978 1.00 44.92 B 116.761 85.577 43.978 1.00 44.92 B 116.761 85.577 43.978 1.00 48.26 B 117.198 83.291 45.361 1.00 48.26 B 117.908 86.750 45.370 1.00 50.17 B 118.309 86.750 45.370 1.00 50.17 B 18.309 86.750 45.370 1.00 50.19 B 18.429 87.139 43.160 1.00 50.26 B 18.429 87.139 43.160 1.00 50.26 B 18.429 87.139 43.160 1.00 50.99 B 18.8429 88.845 40.99 1.00 50.79 B 18.8449 89.848 45.49 1.00 50.79 B 18.8440 1.00 56.67 B 18	CCCCCOCONCCCOOCONCCCCCONCCONCCCCCCNCONCCCCCC
ATOM 6853	CA ARG 1 CB ARG 1 CG ARG 1 CD ARG 1 NE ARG 1 CZ ARG 1	40 114. 994 89. 838 45. 409 1. 00 57. 44 B	C C C C N C

SUBSTITUTE SHEET (RULE 26)

	FIG. 4-141	(Continued)
ATOM 6860 NH2 ARG 14 ATOM 6861 C ARG 14 ATOM 6862 O ARG 14 ATOM 6863 N GLN 14 ATOM 6864 CA GLN 14 ATOM 6865 CB GLN 14 ATOM 6866 CG GLN 14 ATOM 6866 CG GLN 14 ATOM 6868 OE1 GLN 14 ATOM 6869 NE2 GLN 14 ATOM 6870 C GLN 14 ATOM 6871 O GLN 14 ATOM 6872 N LEU 14 ATOM 6873 CA LEU 14 ATOM 6875 CG LEU 14 ATOM 6875 CG LEU 14 ATOM 6876 CD1 LEU 14 ATOM 6877 CD2 LEU 14 ATOM 6877 CD2 LEU 14 ATOM 6878 C LEU 14 ATOM 6879 O LEU 14 ATOM 6880 N ILE 14 ATOM 6881 CA ILE 14 ATOM 6881 CA ILE 14 ATOM 6882 CB ILE 14 ATOM 6883 CG2 ILE 14 ATOM 6884 CG1 ILE 14 ATOM 6885 CD1 ILE 14 ATOM 6886 C ILE 14 ATOM 6887 O ILE 14 ATOM 6888 N THR 144 ATOM 6889 CA THR 144 ATOM 6890 CB THR 144 ATOM 6891 OG1 THR 144 ATOM 6893 C THR 144 ATOM 6894 O THR 144	116. 507 86. 478 50. 911 1. 00 68. 11 113. 697 90. 537 44. 994 1. 00 56. 16 113. 067 91. 225 45. 795 1. 00 56. 03 1 113. 315 90. 363 43. 733 1. 00 54. 56 1 112. 088 90. 947 43. 205 1. 00 53. 90 1 112. 367 92. 292 42. 522 1. 00 55. 16 1 13. 166 92. 203 41. 227 1. 00 57. 86 1 13. 078 93. 477 40. 400 1. 00 59. 30 1 113. 414 94. 562 40. 875 1. 00 60. 96 1 112. 620 93. 350 39. 158 1. 00 58. 33 1 111. 500 89. 965 42. 198 1. 00 52. 05 1 112. 230 89. 362 41. 418 1. 00 52. 50 1 112. 230 89. 362 41. 418 1. 00 52. 50 1 112. 230 89. 362 41. 418 1. 00 52. 50 1 110. 186 89. 794 42. 213 1. 00 50. 43 2 110. 186 89. 794 42. 213 1. 00 50. 43 2 109. 564 88. 861 41. 284 1. 00 48. 86 2 108. 196 88. 415 41. 815 1. 00 48. 86 2 108. 196 88. 415 41. 815 1. 00 48. 86 2 108. 196 88. 415 41. 815 1. 00 48. 84 2 107. 024 89. 395 41. 857 1. 00 49. 83 2 106. 014 88. 940 42. 905 1. 00 47. 77 2 109. 423 89. 467 39. 896 1. 00 47. 77 2 109. 423 89. 467 39. 896 1. 00 47. 77 2 109. 835 89. 226 37. 520 1. 00 42. 98 2 10. 442 88. 208 36. 535 1. 00 42. 34 2 10. 204 88. 659 35. 099 1. 00 41. 35 2 112. 675 87. 257 35. 755 1. 00 42. 12 2 108. 385 89. 481 37. 131 1. 00 42. 92 2 107. 522 88. 617 37. 292 1. 00 41. 84 2 108. 128 90. 680 36. 620 1. 00 43. 57 2 106. 789 91. 065 36. 202 1. 00 44. 05 2 106. 332 92. 344 36. 915 1. 00 45. 33 2 106. 124 92. 080 38. 388 1. 00 43. 31 2 106. 716 91. 294 34. 701 1. 00 44. 53	B CONCCCCCONCCCCCONCCCCCONCCCCCCCONCCCCCCC
ATOM 6895 N GLU 145 ATOM 6896 CA GLU 145 ATOM 6897 CB GLU 145	107. 802 90. 988 34. 001 1. 00 45. 05 107. 857 91. 168 32. 557 1. 00 46. 88 109. 069 92. 031 32. 202 1. 00 50. 14	B O B N B C B C
ATOM 6898 CG GLU 145 ATOM 6899 CD GLU 145 ATOM 6900 OE1 GLU 145 ATOM 6901 OE2 GLU 145 ATOM 6902 C GLU 145 ATOM 6903 O GLU 145 ATOM 6904 N GLU 146	109. 148 93. 319 33. 007 1. 00 55. 05 110. 429 94. 094 32. 760 1. 00 57. 57 110. 696 94. 443 31. 591 1. 00 60. 26 111. 167 94. 357 33. 737 1. 00 59. 47 107. 946 89. 822 31. 834 1. 00 46. 87 108. 648 88. 916 32. 286 1. 00 46. 76 107. 236 89. 695 30. 714 1. 00 46. 37	B C B O B C B C B O
ATOM 6905 CA GLU 146 ATOM 6906 CB GLU 146 ATOM 6907 CG GLU 146 ATOM 6908 CD GLU 146	107. 241 88. 458 29. 932 1. 00 45. 82 108. 592 88. 284 29. 232 1. 00 46. 20 108. 916 89. 321 28. 163 1. 00 45. 55 108. 011 89. 217 26. 948 1. 00 45. 65	B N B C B C B C B C

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					(Continued)
				FIG. 4-144	
ATOM ATOM	7007 7008	NE1 TRP CZ2 TRP	157 157	113.193 76.650 38.030 1.00 22.01 B 113.317 79.051 37.286 1.00 22.77 B	N C
ATOM	7009	CZ3 TRP	157	114. 445 79. 299 35. 156 1. 00 22. 58 B	C
ATOM	7010 7011	CH2 TRP C TRP	157 157	113. 779 79. 846 36. 270 1. 00 21. 74 B 115. 096 73. 640 33. 153 1. 00 22. 79 B	C C
ATOM ATOM	7011	0 TRP	157	114.789 72.483 32.882 1.00 23.16 B	Ö
ATOM	7013	N SER	158	116.198 74.211 32.697 1.00 21.93 B	Ň
ATOM	7014	CA SER	158	117. 154 73. 441 31. 928 1. 00 22. 68 B	C
ATOM	7015	CB SER	158	118. 104 74. 377 31. 172 1. 00 23. 20 B	C
ATOM	7016	OG SER	158	118.550 75.444 31.996 1.00 22.94 B	0
ATOM ATOM	7017 7018	C SER O SER	158 158	117. 898 72. 667 33. 017 1. 00 23. 12 B 117. 800 73. 006 34. 198 1. 00 23. 58 B	. C
ATOM	7019	N PRO	159	118.641 71.619 32.650 1.00 23.10 B	N N
ATOM	7020	CD PRO	159	118.927 71.096 31.307 1.00 23.69 B	Ĉ
ATOM	7021	CA PRO	159	119. 362 70. 860 33. 679 1. 00 24. 10 B	Ċ
ATOM	7022	CB PRO	159	120. 041 69. 744 32. 886 1. 00 24. 45 B	C
ATOM	7023	CG PRO	159	119. 230 69. 660 31. 599 1. 00 23. 97 B	C
ATOM	7024	C PRO	159	120. 384 71. 738 34. 391 1. 00 25. 41 B	C
ATOM ATOM	7025 7026	O PRO N VAL	159 160	120. 598 71. 619 35. 589 1. 00 26. 39 B 121. 014 72. 619 33. 627 1. 00 27. 71 B	O N
ATOM	7027	CA VAL	160	122.031 73.517 34.146 1.00 29.28 B	Č
ATOM	7028	CB VAL	160	123. 383 73. 272 33. 438 1. 00 30. 65 B	Č
ATOM	7029	CG1 VAL	160	124. 421 74. 249 33. 939 1. 00 33. 70 B	C
ATOM	7030	CG2 VAL	160	123. 844 71. 840 33. 670 1. 00 31. 96 B	C
ATOM	7031	C VAL	160	121. 606 74. 952 33. 885 1. 00 29. 74 B	C
ATOM ATOM	7032 7033	O VAL N GLY	160 161	120. 889 75. 224 32. 923 1. 00 30. 93 B 122. 043 75. 866 34. 745 1. 00 29. 32 B	O N
ATOM	7034	CA GLY	161	121. 706 77. 266 34. 562 1. 00 28. 43 B	C
ATOM	7035	C GLY	161	120. 289 77. 645 34. 944 1. 00 28. 19 B	č
ATOM	7036	0 GLY	161	119.839 77.359 36.053 1.00 30.02 B	Ö
ATOM	7037	N HIS	162	119.584 78.296 34.025 1.00 26.53 B	N
ATOM	7038	CA HIS	162	118. 222 78. 721 34. 290 1. 00 25. 12 B	C
ATOM	7039	CB HIS	162	118. 214 79. 959 35. 177 1. 00 26. 70 B	C
ATOM ATOM	7040 7041	CG HIS	162 162	119.019 81.094 34.629 1.00 29.24 B 118.664 82.148 33.857 1.00 30.20 B	C C
ATOM	7042	ND1 HIS	162	120. 378 81. 208 34. 830 1. 00 29. 95 B	N N
ATOM	7043	CE1 HIS	162	120. 824 82. 283 34. 207 1. 00 30. 75 B	Ċ
ATOM	7044	NE2 HIS	162	119. 804 82. 871 33. 608 1. 00 30. 77 B	N
ATOM	7045	C HIS	162	117. 384 79. 021 33. 059 1. 00 24. 68 B	C
ATOM	7046	O HIS	162	116. 730 80. 061 33. 007 1. 00 24. 17 B	0
ATOM ATOM	7047 7048	N LYS CA LYS	163	117. 406 78. 135 32. 067 1. 00 22. 79 B	N C
ATOM	7049	CB LYS	163 163	116. 575 78. 340 30. 889 1. 00 23. 10 B 117. 113 77. 578 29. 675 1. 00 22. 90 B	C C
ATOM	7050	CG LYS	163	118. 367 78. 184 29. 063 1. 00 23. 40 B	Č
ATOM	7051	CD LYS	163	118. 797 77. 407 27. 841 1. 00 22. 69 B	č
ATOM	7052	CE LYS	163	120. 103 77. 930 27. 282 1. 00 23. 67 B	C
ATOM	7053	NZ LYS	163	120. 616 77. 045 26. 195 1. 00 24. 56 B	N
ATOM	7054	C LYS	163	115. 215 77. 779 31. 266 1. 00 24. 15 B	C
ATOM	7055	0 LYS	163	115. 079 77. 104 32. 282 1. 00 24. 69 B	0

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	•			(Canting 3)
			FIG. 4-145	(Continued)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	7056 N LEU 7057 CA LEU 7058 CB LEU 7059 CG LEU 7060 CD1 LEU 7061 CD2 LEU 7062 C LEU 7063 O LEU 7064 N ALA 7065 CA ALA 7066 CB ALA 7066 CB ALA 7067 C ALA 7068 O ALA 7069 N TYR 7070 CA TYR 7071 CB TYR 7071 CB TYR 7072 CG TYR 7073 CD1 TYR 7074 CE1 TYR 7075 CD2 TYR 7076 CE2 TYR 7077 CZ TYR 7078 OH TYR 7079 C TYR 7070 CA VAL 7080 O TYR 7080 O TYR 7081 N VAL 7082 CA VAL 7083 CB VAL 7084 CG1 VAL 7085 CG2 VAL 7086 C VAL 7087 O VAL 7088 N TRP 7080 CB TRP 7090 CB TRP	164 164 164 164 164 165 165 165 165 166 166 166 166 166 166	114. 210 78. 062 30. 450 1. 00 24. 82 B 112. 870 77. 572 30. 704 1. 00 24. 27 B 111. 991 78. 672 31. 293 1. 00 25. 27 B 112. 216 78. 969 32. 769 1. 00 25. 61 B 111. 420 80. 181 33. 178 1. 00 25. 08 B 111. 802 77. 756 33. 582 1. 00 25. 20 B 112. 231 77. 068 29. 435 1. 00 25. 20 B 112. 438 77. 616 28. 353 1. 00 26. 77 B 112. 438 77. 616 28. 353 1. 00 24. 98 B 110. 736 75. 408 28. 479 1. 00 23. 92 B 111. 408 74. 127 28. 021 1. 00 23. 20 B 109. 394 75. 106 29. 114 1. 00 25. 13 B 109. 326 74. 494 30. 188 1. 00 24. 06 B 107. 016 75. 317 29. 027 1. 00 24. 24 B 106. 576 76. 522 29. 866 1. 00 27. 58 B 106.	CCCCCONCCCONCCCCCCCONCCCCCONCCCCCC
ATOM ATOM ATOM	7093 CE2 TRP 7094 CE3 TRP 7095 CD1 TRP	168 168 168	99. 839 79. 907 24. 763 1. 00 27. 63 B	C
ATOM	7096 NE1 TRP	168	98. 452 79. 526 28. 017 1. 00 27. 81 B	C N
ATOM ATOM	7097 CZ2 TRP 7098 CZ3 TRP	168 168	97. 682 81. 074 26. 194 1. 00 26. 74 B 99. 029 80. 886 24. 189 1. 00 29. 25 B	C C
ATOM ATOM	7099 CH2 TRP 7100 C TRP	168 168	97. 962 81. 456 24. 910 1. 00 28. 86 B	C
ATOM	7101 O TRP	168	100. 072 75. 838 25. 444 1. 00 22. 93 B 100. 577 75. 692 24. 328 1. 00 21. 98 B	C 0
ATOM ATOM	7102 N ASN 7103 CA ASN	169 169	98. 768 75. 705 25. 675 1. 00 21. 44 B	N
ATOM	7104 CB ASN	169	97. 830 75. 350 24. 610 1. 00 22. 01 B 97. 394 76. 580 23. 813 1. 00 23. 30 B	C C
		_		

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				F	FIC	G. 4-	146				(Con	tinued)
ATOM	7105		SN 16		. 682	77. 615	24. 662	1.00		В	C	
ATOM	7106	OD1 A			. 240	78. 640	24. 150	1.00		В	0	
ATOM	7107	ND2 A			. 570	77. 361	25.961	1.00		В	N	
ATOM	7108		ISN 16 ISN 16		. 463 . 455	74. 345 74. 541	23. 655 22. 441	1.00 1.00		B B	0 C	
ATOM ATOM	7109 7110		ISN 10 ISN 17		. 433	73. 283	24. 221	1.00		В	N	
ATOM	7111		ISN 17		. 661	72. 208	23. 459	1.00		В	Č	
ATOM	7112		SN 17		. 615	71.515	22. 592	1.00		B	č	
ATOM	7113		SN 17		. 629	70. 741	23. 412	1.00		В	Č	
ATOM	7114	OD1 A			. 158	71. 224	24. 440	1.00		B	Ö	
ATOM	7115	ND2 A			. 300	69.529	22.966	1.00		В	N	
ATOM	7116		ISN 17	0 100	. 859	72.581	22.598	1.00		В	С	
ATOM	7117		ISN 17		. 194	71.861	21.659	1.00		В	0	
ATOM	7118		ISP 17		. 504	73.697	22.916	1.00		В	N	
ATOM	7119		SP 17	1 102	. 671	74. 122	22. 160	1.00		В	Ç	
ATOM	7120		LSP 17		. 354	75.364	21.334	1.00		В	C	
ATOM	7121		SP 17		. 794	75.017	19. 978	1.00		В	C	
ATOM	7122	OD1 A			. 505	74. 338	19. 210	1.00 1 1.00		В	0	
ATOM	7123 7124	OD2 A			. 650 . 850	75. 415 74. 380	19.679 23.073	1.00		B B	C 0	
ATOM ATOM	7124		ISP 17 ISP 17		. 672	74. 647	24. 264	1.00		В	0	
ATOM	7126		LE 17		. 051	74. 301	22. 508	1.00		В	N	
ATOM	7127		LE 17		. 273	74. 497	23. 281	1.00		В	Č	
ATOM	7128		LE 17		. 353	73. 456	22. 885		23. 64		č	
ATOM	7129	CG2 I			. 480	73.466	23.896	1.00		B	Č	
ATOM	7130	CG1 I			. 743	72.056	22.846	1.00		В	C	
ATOM	7131	CD1 · I		2 107	. 707	70.986	22.374	1.00	23.66	В	С	
ATOM	7132		LE 17		. 878	75.892	23. 129	1.00		В	C	
ATOM	7133		LE 17		. 881	76.474	22.048	1.00		В	0	
ATOM	7134		YR 17		. 389	76.414	24. 236	1.00		В	N	
ATOM	7135		YR 17		. 025	77.720	24. 272	1.00		В	Č	
ATOM	7136		YR 17		. 111	78.760	24. 933	1.00		В	C	
ATOM	7137		YR 17		. 822	79.002	24. 190	1.00 ± 1.00 ±		В	C	
ATOM ATOM	7138 7139	CD1 T CE1 T			. 788 . 599	78. 063 78. 271	24. 226 23. 535	1.00		B B	C C	
ATOM		CD2 T			. 634		23. 439			В	C	
ATOM	7141	CE2 T			. 444	80. 381	22. 740	1.00		В	Č	
ATOM	7142		YR 17		. 432	79. 429	22. 794	1.00		В	č	
ATOM	7143		YR 17		. 258	79.625	22. 103	1.00		B	ŏ	
ATOM	7144		YR 17		. 308	77.592	25.080	1.00		В	Č	
ATOM	7145		YR 17		. 412	76.735	25.960	1.00		В	0	
ATOM	7146	N V	'AL 17	4 110	. 276	78. 451	24. 782	1.00		В	N	
ATOM	7147		AL 17	4 111	. 551	78.443	25. 480	1.00		В	C	
ATOM	7148		AL 17		. 669	77. 855	24. 587	1.00		В	C	
ATOM	7149	CG1 V			. 006	77. 936	25. 303	1.00		В	C	
ATOM	7150	CG2 V			. 351	76.403	24. 231	1.00		В	C	•
ATOM	7151		AL 17		. 953	79.857	25. 887	1.00	00. IO	B B	C	
ATOM ATOM	7152 7153		/AL 17 .YS 17		. 787 . 47 4	80. 804 79. 990	25. 125 27. 099	1.00		В	O N	
111 Out	1100	11 L	'TO II		. TIT	10.000	21.000	1.00		U	11	

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					(Continued)
				FIG. 4-147	(Continued)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	7154 7155 7156 7157 7158 7159 7160 7161 7162 7163 7164 7165 7166 7167 7177 7173 7174 7175 7176 7177 7178 7177 7178 7178 7179 7180 7181 7182 7183 7184 7185 7186 7187	CA LYS CB LYS CG LYS CCD LYS NZ LYS C LYS O LYS N ILE CA ILE CB ILE CG1 ILE CG2 ILE CG1 ILE CG2 ILE CG3 ILE CG4 ILE CG5 ILE CG6 ILE CG GLU CG GLU CCB GLU CCB GLU CCB GLU CCB GLU CCB GLU CCB CCB CCB PRO CCC PRO CCC PRO CCA ASN CCA ASN	175 175 175 175 175 175 175 176 176 176 176 176 177 177 177 177 177	112. 940 81. 269 27. 608 1. 00 28. 47 B 112. 090 81. 725 28. 794 1. 00 28. 38 B 110. 809 82. 428 28. 413 1. 00 29. 46 B 109. 876 82. 551 29. 611 1. 00 32. 27 B 110. 479 83. 384 30. 725 1. 00 31. 57 B 110. 664 84. 791 30. 307 1. 00 33. 57 B 114. 382 81. 107 28. 064 1. 00 28. 80 B 114. 662 80. 355 28. 999 1. 00 28. 36 B 115. 294 81. 813 27. 401 1. 00 28. 58 B 116. 710 81. 764 27. 749 1. 00 28. 19 B 117. 572 82. 363 26. 624 1. 00 27. 21 B 118. 942 82. 730 27. 146 1. 00 27. 38 B 116. 956 82. 528 29. 044 1. 00 29. 36 B 117. 910 82. 251 29. 768 1. 00 <td>Continued) C C C C C C C C C C C C C C C C C C</td>	Continued) C C C C C C C C C C C C C C C C C C
ATOM	7190	OD1 ASN	179	115.419 89.131 31.915 1.00 39.14 B	O
ATOM	7191	ND2 ASN	179	114.437 91.142 31.806 1.00 40.48 B	N
ATOM	7192	C ASN	179	112.573 88.540 30.535 1.00 36.88 B	C
ATOM	7193	O ASN	179	112. 205 89. 650 30. 159 1. 00 38. 11 B 112. 995 87. 608 29. 689 1. 00 35. 31 B 113. 030 87. 875 28. 260 1. 00 34. 44 B 114. 357 87. 417 27. 662 1. 00 35. 92 B	O
ATOM	7194	N LEU	180		N
ATOM	7195	CA LEU	180		C
ATOM	7196	CB LEU	180		C
ATOM	7197	CG LEU	180	115. 621 88. 014 28. 279 1. 00 36. 91 B 116. 828 87. 572 27. 470 1. 00 37. 09 B 115. 522 89. 536 28. 303 1. 00 37. 24 B 111. 898 87. 166 27. 547 1. 00 33. 52 B	C
ATOM	7198	CD1 LEU	180		C
ATOM	7199	CD2 LEU	180		C
ATOM	7200	C LEU	180		C
ATOM	7201	O LEU	180	111.406 86.149 28.015 1.00 32.50 B	O
ATOM	7202	N PRO	181	111.462 87.704 26.400 1.00 34.20 B	N

					FIG. 4-149	(Continued)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	7252 7253 7254 7255 7256 7257 7258 7262 7263 7264 7265 7266 7267 7268 7269 7270 7271 7272 7273 7274 7275 7276 7277 7278 7279 7280 7281 7282 7283 7284 7285 7286 7287 7288 7289 7290	N CAECOCCEC CON CAECOCCEC ON CAECOCCE CON CA	TRP	186 187 187 187 187 187 187 187 187 187 187	F I G. 4 - 1 4 9 104. 266 76. 469 18. 265 1. 00 22. 05 103. 935 75. 179 16. 457 1. 00 24. 88 B 102. 717 75. 876 16. 049 1. 00 25. 32 B 103. 007 76. 767 14. 832 1. 00 25. 43 B 104. 159 77. 694 15. 025 1. 00 25. 95 B 104. 093 79. 092 15. 321 1. 00 26. 73 B 105. 420 79. 548 15. 487 1. 00 26. 07 B 105. 420 79. 548 15. 487 1. 00 26. 07 B 105. 485 77. 367 15. 019 1. 00 26. 93 B 106. 249 78. 474 15. 298 1. 00 26. 69 B 105. 723 80. 878 15. 789 1. 00 24. 50 B 103. 346 81. 332 15. 764 1. 00 26. 71 B 104. 679 81. 751 15. 922 1. 00 25. 13 B 101. 555 74. 941 15. 709 1. 00 26. 00 B 100. 481 75. 402 15. 339 1. 00 27. 74 B 101. 759 73. 636 15. 839 1. 00 26. 63 B 102. 291 70. 836 15. 781 1. 00 26. 63 B 102. 291 70. 836 15. 781 1. 00 26. 63 B 102. 291 70. 836 15. 781 1. 00 26. 63 B 102. 91 70. 836 15. 781 1. 00 26. 92 B 100. 064 72. 827 17. 866 1. 00 26. 92 B 100. 064 72. 827 17. 866 1. 00 26. 92 B 100. 064 72. 827 17. 866 1. 00 26. 92 B 100. 064 72. 827 17. 866 1. 00 26. 92 B 100. 064 72. 827 17. 866 1. 00 26. 92 B 100. 064 72. 827 17. 866 1. 00 26. 92 B 100. 064 72. 827 17. 866 1. 00 26. 92 B 100. 064 72. 827 17. 866 1. 00 27. 13 B 101. 940 71. 697 13. 552 1. 00 25. 34 B 99. 278 72. 491 19. 045 1. 00 27. 32 B 97. 783 72. 645 18. 847 1. 00 27. 15 B 99. 278 72. 491 19. 045 1. 00 27. 15 B 99. 278 72. 491 19. 045 1. 00 27. 32 B 97. 783 72. 645 18. 847 1. 00 28. 44 B 97. 333 73. 673 18. 345 1. 00 30. 95 B 97. 007 71. 636 19. 242 1. 00 27. 83 B 99. 278 72. 491 19. 045 1. 00 27. 15 B 95. 187 71. 381 17. 628 1. 00 29. 55 B 93. 695 71. 294 17. 317 1. 00 31. 55 B 93. 498 71. 031 15. 458 1. 00 39. 17 B 94. 815 70. 731 15. 458 1. 00 39. 17 B 94. 815 70. 731 15. 458 1. 00 25. 87 B 94. 262 71. 299 21. 096 1. 00 25. 87 B 94. 262 71. 299 21. 096 1. 00 25. 87 B 94. 262 71. 299 21. 096 1. 00 25. 87 B 94. 262 71. 299 21. 096 1. 00 25. 67 B 94. 815 70. 731 20. 028 1. 00 26. 671 B 94. 815 70. 731 20. 028 1. 00 26. 671 B 94. 815 70. 731 20. 028 1. 00 26. 671 B 94. 815 70. 731 20. 028 1. 00 26. 671 B 94. 815 70. 731 20. 028 1. 00 26. 671 B 94. 815	(Continued) O N C C C C C C C C C C C C C C C C C
ATOM ATOM ATOM ATOM	7291 7292 7293 7294	OE2 C	GLU GLU GLU GLU	191 191 191 191	90. 752 71. 859 24. 514 1. 00 34. 15 B 90. 111 71. 522 25. 536 1. 00 36. 46 B 90. 551 72. 932 23. 899 1. 00 35. 96 B 92. 849 69. 263 21. 631 1. 00 23. 31 B	C 0 0 C
ATOM ATOM ATOM	7295 7296 7297 7298	O N CA CB	GLU ASP ASP ASP	191 192 192 192	92. 031 69. 280 20. 713 1. 00 20. 17 B 93. 208 68. 157 22. 287 1. 00 23. 70 B 92. 707 66. 811 21. 996 1. 00 24. 98 B 91. 183 66. 733 22. 149 1. 00 27. 27 B	O N C C
ATOM ATOM		CG OD1	ASP ASP	192 192	90. 700 67. 200 23. 508 1. 00 30. 85 B 91. 335 66. 855 24. 533 1. 00 32. 45 B	C 0

				FIC 4-150	(Continued)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	7301 7302 7303 7304 7305 7306 7307 7308 7309 7310 7311 7312 7313 7314 7315 7316	O ASP N ILE CA ILE CB ILE CG1 ILE CD1 ILE C ILE O ILE N ILE CA ILE CB ILE CG2 ILE CG2 ILE CG1 ILE	192 192 192 193 193 193 193 193 193 194 194 194 194	FIG. 4 - 150 89. 671 67. 908 23. 548 1. 00 32. 44 B 93. 072 66. 329 20. 602 1. 00 25. 95 B 92. 431 65. 426 20. 065 1. 00 27. 81 B 94. 091 66. 926 20. 000 1. 00 25. 46 B 94. 485 66. 512 18. 665 1. 00 25. 50 B 93. 970 67. 502 17. 595 1. 00 26. 97 B 94. 426 67. 057 16. 212 1. 00 26. 11 B 92. 441 67. 552 17. 621 1. 00 27. 90 B 91. 784 66. 246 17. 210 1. 00 29. 23 B 95. 994 66. 390 18. 546 1. 00 25. 04 B 96. 519 65. 297 18. 334 1. 00 26. 34 B 96. 691 67. 510 18. 682 1. 00 22. 43 B 98. 139 67. 505 18. 589 1. 00 21. 47 B 98. 618 68. 429 17. 456 1. 00 21. 58 B 100. 146 68. 414 17. 377 1. 00 18. 60 B 97. 972 68. 001 16. 133 1. 00 19. 45	(Continued) 0 C 0 N C C C C C C C C C C C C C C C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	7317 7318 7319 7320 7321 7322 7323 7324 7325 7326 7327 7328 7329 7330	CD1 ILE C ILE O ILE N TYR CA TYR CB TYR CC TYR CD1 TYR CC1 TYR CC2 TYR CC2 TYR CC2 TYR CC TYR CC TYR CC TYR CC TYR CC TYR	194 194 195 195 195 195 195 195 195 195	98. 331 66. 613 15. 678 1. 00 15. 81 B 98. 779 67. 968 19. 895 1. 00 21. 61 B 98. 544 69. 095 20. 337 1. 00 22. 13 B 99. 580 67. 095 20. 508 1. 00 19. 09 B 100. 272 67. 429 21. 750 1. 00 18. 17 B 100. 079 66. 331 22. 798 1. 00 20. 45 B 98. 647 65. 941 23. 094 1. 00 21. 37 B 97. 873 65. 269 22. 146 1. 00 20. 38 B 96. 584 64. 846 22. 445 1. 00 20. 38 B 98. 087 66. 187 24. 349 1. 00 21. 55 B 96. 797 65. 768 24. 659 1. 00 20. 75 B 96. 052 65. 094 23. 705 1. 00 20. 48 B 94. 785 64. 650 24. 020 1. 00 19. 77 B 101. 771 67. 579 21. 503 1. 00 18. 27 B	C C C C C C C C C C C C C C C C C C C
ATOM ATOM ATOM	7331 7332 7333 7334 7335 7336 7337 7338 7340 7341 7342 7343 7344 7345 7346 7347 7348 7349	O TYR N ASN CA ASN CB ASN CG ASN OD1 ASN ND2 ASN C ASN O ASN N GLY CA GLY C GLY O GLY N ILE CA ILE CB ILE CG2 ILE CG1 ILE CD1 ILE	195 196 196 196 196 196 196 197 197 197 197 198 198 198 198	102. 412 66. 677 20. 967 1. 00 19. 50 B 102. 334 68. 710 21. 897 1. 00 17. 52 B 103. 762 68. 941 21. 725 1. 00 17. 79 B 104. 011 70. 187 20. 867 1. 00 17. 21 B 103. 366 70. 106 19. 489 1. 00 17. 04 B 103. 769 69. 311 18. 632 1. 00 16. 41 B 102. 362 70. 943 19. 267 1. 00 17. 01 B 104. 380 69. 160 23. 104 1. 00 18. 89 B 103. 976 70. 066 23. 828 1. 00 21. 80 B 105. 355 68. 344 23. 479 1. 00 18. 21 B 105. 976 68. 533 24. 778 1. 00 18. 42 B 105. 185 67. 948 25. 941 1. 00 18. 43 B 103. 976 67. 469 25. 654 1. 00 15. 16 B 103. 129 66. 842 26. 667 1. 00 <td>O N C C O N C C C C C C C C C C C</td>	O N C C O N C C C C C C C C C C C

		FIG. 4-151	(Continued)
ATOM 7350 ATOM 7351 ATOM 7352 ATOM 7353 ATOM 7353 ATOM 7354 ATOM 7355 ATOM 7356 ATOM 7356 ATOM 7357 ATOM 7363 ATOM 7363 ATOM 7363 ATOM 7363 ATOM 7363 ATOM 7363 ATOM 7366 ATOM 7366 ATOM 7366 ATOM 7366 ATOM 7367 ATOM 7370 ATOM 7370 ATOM 7371 ATOM 7371 ATOM 7372 ATOM 7373 ATOM 7373 ATOM 7373 ATOM 7374 ATOM 7376 ATOM 7378 ATOM 7380 ATOM 7381 ATOM 7382 ATOM 7383 ATOM 7384 ATOM 7385 ATOM 7386 ATOM 7386 ATOM 7387 ATOM 7388 ATOM 7388	C ILE 19 O ILE 19 N THR 19 CA THR 19 CB THR 19 CG2 THR 19 CG2 THR 19 CG3 THR 19 CG4 ASP 20 CG ASP 20 CG ASP 20 OD1 ASP 20 OD2 ASP 20 OD2 ASP 20 OD2 ASP 20 OD2 ASP 20 CA TRP 20 CA TRP 20 CA TRP 20 CB TRP 20 CCB TRP 20 CCB TRP 20 CCCB TRP 20 CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC	8 102.354 65.447 24.895 1.00 16.78 B 9 102.182 64.671 26.990 1.00 15.77 B 9 101.600 63.396 26.608 1.00 15.94 B 9 101.982 62.350 27.630 1.00 15.69 B 9 101.683 62.861 28.937 1.00 12.99 B 9 103.473 62.043 27.534 1.00 15.54 B 9 100.085 63.448 26.522 1.00 15.87 B 9 100.085 63.448 26.522 1.00 16.77 B 99.510 62.534 25.745 1.00 16.29 B 0 98.058 62.450 25.619 1.00 16.42 B 0 97.654 61.812 24.279 1.00 17.56 B 0 97.654 61.812 24.207 1.00 19.40 B 0 97.657 61.578 26.806 1.00 19.79 B 0 97.657 61.578 26.890 1.00 19.79 B	CONCCOCCONCCCOOCONCCCCCONCCCCONCCCCONCCCCONCCCCONCCCCONCCCCONCCCCONCCCCONCCCCCONCCCCCONCCCCCONCCCCCONCCCCCC
ATOM 7389 ATOM 7390	N TYR 20 CA TYR 20 CB TYR 20	99. 616 57. 857 26, 906 1. 00 15. 45 B 101. 060 57. 941 27. 053 1. 00 13. 39 B	
ATOM 7391 ATOM 7392 ATOM 7393 ATOM 7394	CG TYR 200 CD1 TYR 200 CE1 TYR 200 CD2 TYR 200	B 102. 248 58. 238 24. 823 1. 00 8. 90 B 101. 461 57. 938 23. 709 1. 00 8. 82 B 101. 989 57. 260 22. 619 1. 00 7. 48 B	C C C C
ATOM 7395 ATOM 7396 ATOM 7397 ATOM 7398	CE2 TYR 203 CZ TYR 203 OH TYR 203 C TYR 203	104.128 57.167 23.727 1.00 6.51 B 103.325 56.874 22.634 1.00 8.49 B 103.849 56.175 21.572 1.00 8.01 B	C C O C

										(Continued)
					FIC	3.4-	1 5 2			(Oomania a)
ATOM	7399	0	TYR	203	102. 369	57.832	29.056	1.00 12.65	. В	0 .
ATOM	7400	Ň	GLU	204	100. 706	59. 335	29.020	1.00 15.26	В	Ň
ATOM	7401	CA	GLU	204	100.963	59.827	30.376	1.00 16.69	В	С
ATOM	7402	CB	GLU	204	99.975	60.936	30.743	1.00 16.67	В	C
ATOM	7403	CG	GLU	204	100.174	61.457	32.161	1.00 17.47	В	.C
ATOM	7404	CD	GLU	204	98.950	62.154	32.731	1.00 17.71	В	С
ATOM	7405	0E1	GLU	204	98. 197	62.785	31.964	1.00 19.00	В	0
ATOM	7406		GLU	204	98. 753	62.085	33.962	1.00 18.59	В	0
ATOM	7407	С	GLU	204	100.831	58.740	31. 437	1.00 17.37	В	C
ATOM	7408	0	GLU	204	101.681	58. 597	32.305	1.00 18.22	В	0
MOTA	7409	N	GLU	205	99. 745	57.980	31. 353	1.00 18.89	В	N
ATOM	7410	CA	GLU	205	99.442	56.932	32. 315	1.00 19.55	В	C
ATOM	7411	CB	GLU	205	97. 925	56.727	32. 344	1.00 20.80	В	C
ATOM	7412	CG	GLU	205	97. 453	55. 436	32. 995	1.00 23.74	В	C
ATOM	7413	CD	GLU	205	97.414	55.494	34. 515	1.00 26.68	В	C
ATOM	7414	0E1		205	97. 038	54.466	35. 118	1.00 28.71	B B	0 0
ATOM	7415	OE2 C	GLU GLU	205 205	97. 744 100. 132	56. 547 55. 578	35. 106 32. 131	1.00 26.12 1.00 19.27	В	C
ATOM ATOM	7416 7417	0	GLU	205 205	100. 132	54. 957	33. 107	1.00 19.21	В	0
ATOM	7418	N	GLU	206	100. 323	55. 124	30. 893	1.00 13.31	В	N
ATOM	7419	CA	GLU	206	100. 231	53.808	30.660	1.00 18.63	В	C
ATOM	7420	CB	GLU	206	99. 989	53.016	29. 705	1.00 18.05	B	Č
ATOM	7421	CG	GLU	206	98. 535	52.921	30. 139	1.00 20.39	B	Č
ATOM	7422	CD	GLU	206	98. 359	52.143	31.422	1.00 20.74	B	C C
ATOM	7423		GLU	206	97. 205	51.905	31. 821	1.00 21.45	B	Ö
ATOM	7424		GLU	206	99.375	51.768	32.037	1.00 22.90	В	0
ATOM	7425	C	GLU	206	102.293	53.766	30.136	1.00 19.32	В	C
ATOM	7426	0	GLU	206	102.976	52.761	30. 292	1.00 20.01	В	0
ATOM	7427	N	VAL	207	102.744	54.844	29.509	1.00 20.90	В	N
ATOM	7428	CA	VAL	207	104. 092	54.855	28. 968	1.00 20.95	В	C
ATOM	7429	CB	VAL	207	104. 101	55. 347	27. 509	1.00 21.52	В	C
ATOM	7430		VAL	207	105.486	55. 151	26. 918	1.00 22.17	В	С
ATOM	7431		VAL	207	103. 048	54. 592	26. 684	1.00 19.10	В	C
ATOM	7432	C	VAL	207	105. 080	55.691	29. 775	1.00 21.67	В	C
ATOM	7433	0	VAL	207	106.052	55. 160	30. 301	1.00 25.32	В	0
ATOM	7434	N	PHE	208	104. 833	56.989	29. 888	1.00 21.55	В	N
ATOM	7435	CA	PHE	208	105.743	57. 870	30.611	1.00 21.33	В	C
ATOM	7436	CB	PHE	208	105.877	59. 201	29. 863	1.00 21.28	В	C
ATOM	7437	CG	PHE	208	106.571	59.083	28. 536	1.00 21.92	В	C
ATOM	7438		PHE PHE	208 208	107. 890 105. 893	58. 649 59. 373	28. 464 27. 353	1.00 20.63 1.00 22.58	B B	C C
ATOM ATOM	7439 7440		PHE	208	103. 693	58. 499	27. 230	1.00 22.52	В	C
ATOM	7441		PHE	208	106. 521	59. 225	26. 109	1.00 22.32	В	C
ATOM	7442	CZ	PHE	208	100. 321	58. 787	26. 048	1.00 22.24	В	C
ATOM	7443	C	PHE	208	107. 657	58. 168	32. 082	1.00 21.89	В	č
ATOM	7444	ŏ	PHE	208	106. 298	58. 727	32. 768	1.00 23.07	B	ŏ
ATOM	7445	N	SER	209	104. 261	57.811	32. 577	1.00 20.48	B	Ň
ATOM	7446	ĊA	SER	209	103. 922	58. 094	33. 976	1.00 19.86	B	Ċ
ATOM	7447	CB	SER	209	104. 689	57. 165	34. 905	1.00 18.09	B	č

									(Continued)
					FIG. 4-1	53			,
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	7448 7449 7450 7451 7452 7453 7454 7455 7456 7457 7458	OG C O N CA CB C O N CA	SER SER SER ALA ALA ALA ALA TYR TYR TYR	209 209 209 210 210 210 210 211 211	104. 383 55. 820 3 104. 285 59. 543 3 104. 780 59. 877 3 104. 031 60. 394 3 104. 319 61. 809 3 105. 809 62. 044 3 103. 545 62. 492 3 103. 042 61. 835 3 103. 461 63. 813 3 102. 733 64. 634 3 101. 944 65. 681 3	34. 601 34. 286 35. 367 33. 302 33. 393 33. 228 32. 275 31. 367 32. 354 31. 390 32. 175	1. 00 21. 42 1. 00 20. 55 1. 00 19. 53 1. 00 20. 69 1. 00 20. 47 1. 00 20. 63 1. 00 20. 53 1. 00 19. 81 1. 00 21. 78 1. 00 20. 95 1. 00 18. 35	B B B B B B B B B B B B B B B B B B B	0 C O N C C C O N
ATOM ATOM	7459 7460	CG CD1	TYR TYR	211 211			1.00 15.38 1.00 14.13	B B	C C
ATOM	7461	CE1	TYR	211	99.310 66.879 2	9.694	1.00 12.47	В	C
ATOM	7462	CD2		211			1.00 11.95	В	C
ATOM ATOM	7463 7464	CE2 CZ	TYR	211 211			1.00 12.21 1.00 13.68	B B	C C
ATOM	7465	OH	TYR	211			1.00 12.73	В	Ö
ATOM	7466	C	TYR	211	103.781 65.283 3	0. 508	1.00 22.11	В	C
ATOM	7467	0	TYR	211			1.00 23.55	В	0
ATOM ATOM	7468 7469	N CA	SER SER	212 212			1.00 23.17 1.00 22.03	B B	N C
ATOM	7470	CB	SER	212			1.00 22.03	В	Č
ATOM	7471	0G	SER	212	108.441 66.477 3	0.567	1.00 24.83	B	Ö
ATOM	7472	C	SER	212			1.00 22.20	В	C
ATOM	7473	0	SER	212			1.00 22.93	В	0
ATOM ATOM	7474 7475		ALA ALA	213 213			1.00 22.14 1.00 19.72	B B	N C
ATOM	7476		ALA	213			1.00 19.85	В	č
ATOM	7477		ALA	213			1.00 21.17	B	č
MOTA	7478		ALA	213			1.00 20.14	В	0
ATOM	7479		LEU	214			1.00 21.21	В	N
ATOM ATOM	7480 7481		LEU LEU	214 214			1.00 22.06 1.00 21.02	B B	C C
ATOM	7482		LEU	214			1.00 21.02	В	Č
ATOM	7483	CD1	LEU	214	108. 840 70. 872 27	7. 603	1.00 21.72	B	č
ATOM	7484	CD2		214			1.00 22.01	В	С
ATOM	7485		LEU	214			1.00 22.30	В	C
ATOM ATOM	7486 7487		LEU TRP	214 215			1.00 25.61 1.00 21.71	B B	0 · N
ATOM	7488		TRP	215			1.00 19.34	В	C
ATOM	7489	CB	TRP	215			1.00 18.71	B	č
ATOM	7490		TRP	215			1.00 18.43	В	C
ATOM	7491	CD2		215			1.00 16.56	В	C
ATOM ATOM	7492 7493	CE2 CE3		215 215			1.00 14.85 1.00 17.01	B B	C C
ATOM	7494	CD1		215			1.00 17.01	В	C
ATOM	7495	NE1	TRP	215	111.781 62.356 28	8. 400	1.00 13.49	В	N
ATOM	7496	CZ2	TRP	215	109.996 61.949 26	6. 682 1	1.00 14.75	В	С

				(Continued)
			FIG. 4-154	(Committee)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	7497 CZ3 TRP 7498 CH2 TRP 7499 C TRP 7500 O TRP 7501 N TRP 7502 CA TRP 7503 CB TRP 7504 CG TRP 7505 CD2 TRP 7506 CE2 TRP 7507 CE3 TRP 7508 CD1 TRP 7509 NE1 TRP 7510 CZ2 TRP 7511 CZ3 TRP 7512 CH2 TRP 7512 CH2 TRP 7513 C TRP 7513 C TRP 7514 O TRP 7515 N SER 7516 CA SER 7517 CB SER 7516 CA SER 7517 CB SER 7518 OG SER 7519 C SER 7518 OG SER 7519 C SER 7510 O SER 7520 O SER 7521 N PRO 7522 CD PRO 7523 CA PRO 7524 CB PRO 7524 CB PRO 7525 CG PRO 7526 C PRO 7526 C PRO 7527 O PRO 7528 N ASN 7529 CA ASN 7529 CA ASN 7530 CB	218 218 218 218 218 219 219	110. 326	Continued) C C C C C C C C C C C C C C C C C C
ATOM ATOM ATOM	7530 CB ASN 7531 CG ASN 7532 OD1 ASN	219 219 219	125. 485 71. 562 28. 816 1. 00 26. 61 B 125. 447 71. 640 27. 308 1. 00 27. 23 B 124. 376 71. 725 26. 706 1. 00 25. 21 B	C C O
ATOM ATOM ATOM ATOM	7533 ND2 ASN 7534 C ASN 7535 O ASN 7536 N GLY	219 219	126.626 71.632 26.690 1.00 30.87 B 123.029 72.133 28.958 1.00 27.38 B 123.212 73.351 28.943 1.00 29.12 B 121.888 71.575 28.565 1.00 26.98 B	N C O N
ATOM ATOM ATOM	7537 CA GLY 7538 C GLY 7539 O GLY	220 220 220	120. 765 72. 391 28. 137 1. 00 26. 30 B 120. 823 73. 030 26. 765 1. 00 26. 91 B 120. 097 73. 986 26. 500 1. 00 27. 55 B	C C O
ATOM ATOM ATOM ATOM	7540 N THR 7541 CA THR 7542 CB THR 7543 OG1 THR	221 221	121. 669 72. 512 25. 884 1.00 27. 00 B 121. 775 73. 073 24. 547 1.00 26. 99 B 123. 052 72. 584 23. 808 1.00 27. 74 B 124. 212 73. 084 24. 481 1.00 27. 74 B	N C C
ATOM ATOM	7544 CG2 THR 7545 C THR	221	124. 213 73. 084 24. 481 1. 00 29. 49 B 123. 068 73. 089 22. 367 1. 00 26. 25 B 120. 559 72. 685 23. 730 1. 00 26. 42 B	0 C C

ATOM 7546 0 THR 221 119.862 73.551 23.201 1.00 28.29 B O ATOM 7547 N PHE 222 120.305 71.386 23.619 1.00 25.34 B N ATOM 7548 CA PHE 222 119.158 70.921 22.850 1.00 25.13 B C ATOM 7549 CB PHE 222 119.480 69.645 22.069 1.00 25.65 B C ATOM 7550 CG PHE 222 110.722 69.723 21.246 1.00 26.35 B C ATOM 7551 CD1 PHE 222 121.955 69.384 21.797 1.00 26.35 B C ATOM 7551 CD1 PHE 222 121.955 69.384 21.797 1.00 26.35 B C ATOM 7551 CD1 PHE 222 121.955 69.384 21.797 1.00 26.35 B C ATOM 7552 CD2 PHE 222 123.616 70.111 19.912 1.00 28.19 B C ATOM 7554 CB2 PHE 222 123.15 69.425 21.031 1.00 28.19 B C ATOM 7555 CC PHE 222 123.163 69.425 21.031 1.00 28.19 B C ATOM 7555 CC PHE 222 121.815 70.158 19.132 1.00 28.19 B C ATOM 7555 CD PHE 222 117.949 70.618 23.723 1.00 28.19 B C ATOM 7556 C PHE 222 118.666 70.282 24.901 1.00 28.46 B C ATOM 7557 O PHE 222 118.666 70.282 24.901 1.00 24.38 B O ATOM 7559 CA LEU 223 115.540 70.442 23.788 1.00 22.85 B C ATOM 7560 CB LEU 223 115.540 70.442 23.788 1.00 22.85 B C ATOM 7560 CB LEU 223 113.469 70.442 23.788 1.00 22.85 B C ATOM 7560 CB LEU 223 113.489 70.684 23.878 1.00 22.85 B C ATOM 7560 CB LEU 223 113.489 70.684 23.878 1.00 22.85 B C ATOM 7560 CB LEU 223 114.618 71.667 23.878 1.00 24.19 B N ATOM 7560 CB LEU 223 114.618 71.667 23.878 1.00 23.33 B C ATOM 7566 CD LEU 223 114.462 69.560 21.808 1.00 23.23 B C ATOM 7566 CD LEU 223 114.462 69.560 21.808 1.00 23.23 B C ATOM 7567 CA ALA 224 114.834 68.162 23.459 1.00 23.37 B C ATOM 7567 CA ALA 224 114.834 68.162 23.459 1.00 23.37 B C ATOM 7567 CA ALA 224 114.834 68.162 23.459 1.00 23.37 B C ATOM 7567 CA ALA 224 114.834 68.162 23.459 1.00 23.37 B C ATOM 7567 CA ALA 224 114.834 68.162 23.459 1.00 23.37 B C ATOM 7570 O ALA 224 112.948 67.111 24.444 1.00 23.37 B C ATOM 7570 O ALA 224 112.948 67.111 24.444 1.00 18.56 B C ATOM 7570 CA TR 225 109.648 68.87 22.703 1.00 21.31 B C ATOM 7570 CA TR 225 109.648 68.87 22.703 1.00 21.31 B C ATOM 7570 CA TR 225 109.648 68.89 20.509 1.00 18.56 B C ATOM 7578 CB TR 225 109.648 68.89 20.509 1.00 18.56 B C ATOM 7588 CA ATOM 7580 CB					FIC	G. 4-	155			(Continued)
ATOM 7589 CA GLN 227 104.659 64.968 19.457 1.00 17.01 B C ATOM 7590 CB GLN 227 104.823 65.709 18.139 1.00 17.47 B C ATOM 7591 CG GLN 227 103.512 66.300 17.670 1.00 18.65 B C ATOM 7592 CD GLN 227 103.554 66.788 16.249 1.00 18.45 B C	ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	7547 N 7548 CA 7549 CB 7550 CG 7551 CD 7552 CD 7553 CE 7554 CE 7555 CZ 7556 C 7557 O 7558 N 7559 CA 7563 CD 7563 CD 7564 C 7565 O 7566 N 7567 CA 7568 CB 7567 CA 7568 CB 7567 CA 7568 CB 7570 O 7571 N 7572 CA 7573 CB 7574 CG 7575 CD 7576 CE 7577 CD 7578 CE 7577 CD	PHE PHE PHE LEUU LEU LALA ALA ATYRR TYRR ALA ALA ALA ALA ALA ALA ALA ALA ALA A	222 222 222 222 222 222 222 222 222 22	119. 862 120. 305 119. 158 119. 480 120. 722 121. 955 120. 661 123. 115 121. 815 123. 046 117. 949 118. 066 116. 780 115. 540 114. 618 113. 248 114. 839 114. 885 114. 885 114. 834 114. 201 114. 935 112. 761 112. 498 111. 825 110. 423 109. 733 109. 648 110. 680 110. 607 108. 543 109. 705 110. 143 109. 705 110. 143 109. 705 110. 143 109. 705 110. 143 109. 705 110. 143 107. 485 106. 528 106. 528 106. 528 107. 107	73. 551 71. 386 70. 921 69. 645 69. 723 69. 384 70. 111 69. 425 70. 746 70. 618 70. 282 70. 746 70. 684 72. 587 69. 810 70. 684 72. 587 69. 650 68. 162 67. 062 67. 062 67. 062 67. 063 67. 111 66. 755 66. 635 67. 997 68. 624 69. 443 70. 017 68. 399 68. 970 69. 777 70. 342 65. 712 65. 723 65. 723 65. 723 65. 723 65. 724 65. 725 65. 726 65. 726 65. 727 66. 988 67. 727 68. 997 68. 997 70. 342 65. 723 65. 72	23. 201 23. 619 22. 850 22. 069 21. 246 21. 797 19. 912 21. 031 19. 132 19. 693 23. 723 24. 901 23. 119 23. 789 23. 878 24. 503 25. 860 24. 644 22. 934 21. 808 23. 459 22. 753 23. 248 24. 444 22. 328 22. 703 22. 701 21. 332 22. 701 21. 332 22. 703 22. 701 21. 332 22. 703 22. 701 21. 332 22. 703 22. 703 22. 701 21. 332 20. 849 19. 589 20. 509 19. 244 18. 796 17. 553 21. 737 20. 607 22. 195 21. 381 22. 173 20. 962 21. 576	1. 00 25. 34 1. 00 25. 65 1. 00 26. 36 1. 00 26. 35 1. 00 26. 35 1. 00 25. 81 1. 00 26. 12 1. 00 28. 19 1. 00 28. 46 1. 00 24. 55 1. 00 24. 38 1. 00 24. 19 1. 00 21. 81 1. 00 20. 49 1. 00 21. 81 1. 00 23. 23 1. 00 23. 23 1. 00 23. 23 1. 00 23. 38 1. 00 23. 37 1. 00 23. 38 1. 00 24. 27 1. 00 23. 38 1. 00 23. 37 1. 00 23. 38 1. 00 24. 27 1. 00 23. 38 1. 00 24. 27 1. 00 23. 38 1. 00 24. 27 1. 00 23. 38 1. 00 18. 49 1. 00 18. 23 1. 00 18. 23 1. 00 18. 23 1. 00 18. 23 1. 00 18. 56 1. 00 16. 52 1. 00 13. 07 1. 00 16. 18 1. 00 14. 89 1. 00 12. 68 1. 00 14. 06 1. 00 21. 55 1. 00 22. 86 1. 00 19. 66 1. 00 19. 73 1. 00 21. 22	B B B B B B B B B B B B B B B B B B B	ONCCCCCCCONCCCCCONCCCCONCCCCCCCCONCCCCO
ATOM 7593 OE1 GLN 227 103.724 66.007 15.320 1.00 18.91 B O ATOM 7594 NE2 GLN 227 103.394 68.090 16.070 1.00 19.57 B N	ATOM ATOM ATOM ATOM ATOM	7589 CA 7590 CB 7591 CG 7592 CD 7593 OE1	GLN GLN GLN GLN GLN	227 227 227 227 227	104. 659 104. 823 103. 512 103. 554 103. 724	64. 968 65. 709 66. 300 66. 788 66. 007	19. 457 18. 139 17. 670 16. 249 15. 320	1. 00 17. 01 1. 00 17. 47 1. 00 18. 65 1. 00 18. 45 1. 00 18. 91	B B B B	C C C O

										(Continued)
				•	FIG	. 4 -	156			(Continued)
ATOM	7595	C	GLN	227		63. 841	19. 274	1.00 17.21	В	C
ATOM	7596	0	GLN	227		62.850	18. 594	1.00 17.76	В	0
ATOM	7597	N	PHE	228		63. 990	19. 888	1.00 16.03	В	N C
ATOM	7598	CA	PHE	228		62. 980	19. 768	1.00 17.64 1.00 14.78	B B	C C
ATOM	7599	CB	PHE	228 228		62. 524 62. 105	21. 158 22. 065	1.00 14.78	В	Č
MOTA	7600	CG	PHE PHE	228		63. 003	22. 982	1.00 13.03	В	Č
ATOM ATOM	7601 7602		PHE	228		60. 826	21. 978	1.00 12.01	В	č
ATOM	7603		PHE	228		62.636	23. 796	1.00 9.77	В	č
ATOM	7604		PHE	228		60.450	22. 786	1.00 11.27	B	č
ATOM	7605	CZ	PHE	228		61.360	23.698	1.00 9.50	B	Č
ATOM	7606	Č	PHE	228	100.263	63. 523	18.955	1.00 18.96	В	C
ATOM	7607	Ŏ	PHE	228		64.697	19.064	1.00 19.98	В	0
ATOM	7608	N	ASN	229		62.657	18. 133	1.00 20.11	В	N
ATOM	7609	CA	ASN	229		63.002	17. 285	1.00 20.74	В	С
ATOM	7610	CB	ASN	229		62.867	15.819	1.00 22.98	В	C
ATOM	7611	CG	ASN	229		63. 488	14.867	1.00 27.56	В	C
ATOM	7612		ASN	229		63. 610	15. 174	1.00 31.63	В	0
ATOM	7613		ASN	229		63. 871	13. 692	1.00 30.76	В	N
ATOM	7614	C	ASN	229		61.995	17. 609	1.00 21.10	В	C
ATOM	7615	0	ASN	229		60.816	17. 283	1.00 20.02 1.00 22.16	В	0 N
ATOM ATOM	7616	N CA	ASP ASP	230 230		62. 444 61. 534	18. 260 18. 608	1.00 24.10	B B	N C
ATOM	7617 7618	CB	ASP	230		61. 683	20.079	1.00 24.31	В	Č
ATOM	7619	CG	ASP	230		61.332	21.027	1.00 25.00	В	Č
ATOM	7620		ASP	230		60. 914	22. 159	1.00 27.89	B	ŏ
ATOM	7621		ASP	230		61.485	20.656	1.00 27.78	B	Ŏ.
ATOM	7622	Č	ASP	230		61.776	17.740	1.00 24.83	B	Č
MOTA	7623	0	ASP	230		61.496	18.148	1.00 24.00	В	0
ATOM	7624	N	THR	231		62. 284	16.536	1.00 25.37	В	N
ATOM	7625	CA	THR	231		62. 582	15. 593	1.00 26.24	В	C
ATOM	7626	CB	THR	231		62.868	14. 193	1.00 25.71	В	C
ATOM	7627	0G1		231		64. 151	14. 194	1.00 26.78	В	0
ATOM	7628		THR	231		62. 851	13. 150	1.00 23.72	В	C
ATOM	7629	C	THR	231		61.510	15. 467	1.00 27.04	В	C
ATOM	7630	0	THR	231		61.815	15.604	1.00 29.05	В	0
ATOM	7631 7632	N CA	GLU GLU	232 232		60. 265 59. 183	15. 211 15. 038	1.00 27.00 1.00 26.30	В	Ŋ
ATOM ATOM	7633	CB	GLU	232 232		58. 286	13. 877	1.00 20.30	B B	C C
ATOM	7634	CG	GLU	232		59. 036	12. 563	1.00 25.71	В	Ċ
ATOM	7635	CD	GLU	232		58. 253	11.519	1.00 39.94	В	č
ATOM	7636	0E1		232		57. 273	10. 943	1.00 41.61	В	ŏ
ATOM	7637		GLU	232		58. 623	11. 286	1.00 39.28	B	ŏ
ATOM	7638	Č	GLU	232		58. 328	16. 282	1.00 23.78	B	č
ATOM	7639	Ö	GLU	232		57. 280	16. 208	1.00 23.18	B	0
ATOM	7640	N	VAL	233	91.823	58. 763	17.427	1.00 21.91	В	N
ATOM	7641	CA	VAL	233		58.010	18.652	1.00 20.18	В	C
ATOM	7642	CB	VAL	233		58. 375	19.727	1.00 20.26	В	C
ATOM	7643	CG1	VAL	233	92. 352	57. 627	21.016	1.00 18.23	В	С

	FIG. 4-157	(Continued)
ATOM 7644 CG2 VAL ATOM 7645 C VAL ATOM 7646 O VAL ATOM 7647 N PRO ATOM 7648 CD PRO ATOM 7654 CG PRO ATOM 7650 CB PRO ATOM 7651 CG PRO ATOM 7652 C PRO ATOM 7653 O PRO ATOM 7654 N LEI ATOM 7656 CB LEI ATOM 7656 CB LEI ATOM 7656 CB LEI ATOM 7657 CG LEI ATOM 7658 CD1 LEI ATOM 7660 C LEI ATOM 7661 O LEI ATOM 7663 CA ILEI ATOM 7663 CA ILEI ATOM 7666 CG1 ILEI ATOM 7667 CD1 ILEI ATOM 7668 C ILEI ATOM 7669 O ILEI ATOM 7669 O ILEI ATOM 7670 N GLU ATOM 7671 CA GLU ATOM 7671 CA GLU ATOM 7672 CB GLU ATOM 7673 CG GLU ATOM 7674 CD GLU ATOM 7675 OE1 GLU ATOM 7676 OE2 GLU ATOM 7677 C GLU ATOM 7678 O GLU ATOM 7679 N TYR ATOM 7680 CA TYR ATOM 7681 CB TYR ATOM 7683 CD1 TYR ATOM 7684 CE1 TYR ATOM 7685 CD2 TYR ATOM 7685 CD2 TYR ATOM 7686 CE2 TYR	2 233 94.050 58.032 19.223 1.00 18.80 2 233 90.218 58.339 19.175 1.00 18.04 2 233 89.886 59.507 19.378 1.00 19.49 2 234 89.383 57.315 19.394 1.00 14.37 2 234 88.0633 55.876 19.231 1.00 14.37 2 234 88.025 57.544 19.896 1.00 15.33 2 234 88.247 55.363 19.013 1.00 12.89 2 234 88.048 58.275 21.227 1.00 14.45 2 234 88.048 58.275 21.227 1.00 14.92 234 89.043 58.242 21.950 1.00 13.13 235 86.911 58.927 21.547 1.00 14.92 235 86.131 61.005 22.536 1.00 14.93 235 86.627 61.937 21.434 1.00 16.83 235 87.963 62.534 21.833 1.00 17.90 235 87.963	B B B B B B B B B B B B B B B B B B B
ATOM 7685 CD2 TYR	238 84.390 60.160 31.291 1.00 14.07	B C

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					F	ì I C	3. 4	-	158				(Continued)
ATOM	7693	СВ	SER	239	77	. 597	62. 78	33	33. 085		13. 29	В		С
ATOM	7694	0G	SER	239		. 800	62. 49		31.961		19.37	В		0
ATOM	7695	C	SER	239		. 775	63. 54		33. 915		14.65	В		C
ATOM	7696	0	SER	239		. 361	62. 77		34. 673		15.52	В		0
ATOM	7697	N	PHE	240		. 737	64. 86		34. 100		14.89	В		N
ATOM	7698	CA	PHE	240		. 313	65. 49		35. 276		15.60	В		C
ATOM	7699	CB	PHE	240		. 543	66. 32		34. 932		17.00	В		C
ATOM	7700	CG	PHE	240		. 422	66. 59		36. 112		14.96	В		C
ATOM	7701		PHE	240		. 325	65. 62		36. 547		15.66	В		C
ATOM	7702		PHE	240		. 312 . 108	67. 78 65. 84		36. 822 37. 675		14.41	В		C
ATOM ATOM	7703 7704		PHE PHE	$\begin{array}{c} 240 \\ 240 \end{array}$. 108	68.00		37. 950		13.32	B B		C C
ATOM	7705	CZ	PHE	240		. 988	67. 03		38. 379		11.23	В		C
ATOM	7706	C	PHE	240		. 184	66. 40		35. 758		15. 75	В		C
ATOM	7707	ŏ	PHE	240		. 671	67. 23		34. 995		14.05	В		Ŏ
ATOM	7708	N	TYR	241		. 785	66. 23		37. 013		15.13	B		N
ATOM	7709	CA	TYR	241		. 683	67.00		37. 567		14. 92	В		C
ATOM	7710	CB	TYR	241		. 912	66. 12		38. 545		13. 15	B		č
ATOM	7711	CG	TYR	241		. 480	64. 84		37. 880		12.77	B		Č
ATOM	7712	CD1		241		. 393	64.83		37.007		11.36	В		Č
ATOM	7713	CE1	TYR	241		. 051	63.67		36. 304		12.47	В		C
ATOM	7714	CD2	TYR	241	77.	. 215	63.67	74	38. 041	1.00	12.85	В		C
ATOM	7715		TYR	241		. 883	62.51		37. 342	1.00	12.55	В		C
ATOM ·	7716	CZ	TYR	241		. 801	62.52		36. 472		12.41	В		C
ATOM	7717	OH	TYR	241		. 489	61.39		35. 748		12.90	В		0
ATOM	7718	C	TYR	241		. 100	68. 29		38. 208		15. 24	В		C
ATOM	7719	0	TYR	241		. 311	69. 23		38. 263		17.04	В		0
ATOM	7720	N	SER	242		. 337	68.35		38. 694		16. 92	В		N
ATOM	7721	CA	SER	242		. 864	69.57		39. 305		16.89	В		C
ATOM	7722	CB	SER	242		. 816	70.70		38. 280		15. 48	В		C
ATOM	7723	OG	SER	242		. 439	71.87		38. 782		18. 12	В		0
ATOM ATOM	7724 7725	C 0	SER SER	242 242		. 078	69.96		40. 548		16.70	В		C
ATOM	7726	N	ASP	242	70	. 438 . 136	69.12 71.24		41.171 40.912	1.00	18. 07 17. 57	B B		0 N
ATOM	7727	CA	ASP	243		. 405	71.72		42. 075		19. 72	. В		N C
ATOM		CB		243					42. 442			В		Č
ATOM	7729	CG	ASP	243		. 275	73. 18		42. 950		28. 70	В		Č
ATOM	7730	0D1		243		646	72.30		43. 765		29. 62	В		0
ATOM	7731	0D2		243		. 021	74. 10		42.542		29.69	В		0
ATOM	7732	C	ASP	243		917	71.70		41.772		20. 24	B		Č
ATOM	7733	Ö	ASP	243		508	71.77		40.609		20. 38	В		Ŏ
ATOM	7734	N	GLU	244		104	71.62		42.818		19. 25	B		Ň
ATOM	7735	CA	GLU	244		668	71.54		42.630		19.29	B		C
ATOM	7736	CB	GLU	244		966	71.37		43.988		19.46	В		Č
ATOM	7737	CG	GLU	244		283	72.60		44. 533		23.65	B		Č
ATOM	7738	CD	GLU	244		567	72.33		45.847		26.30	В		Č
ATOM	7739		GLU	244		225	71.85		46. 797		28.64	В		0
ATOM	7740	0E2		244		349	72.59	5	15.934		27. 72	В		0
ATOM	7741	C	GLU	244	74.	086	72.72	0 4	41.850	1.00	18. 30	В		C

		FIG. 4-159	(Continued)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	7743 N SER 245 7744 CA SER 245 7745 CB SER 245 7746 OG SER 245 7747 C SER 245 7748 O SER 245 7748 N LEU 246 7750 CA LEU 246 7751 CB LEU 246 7751 CB LEU 246 7752 CG LEU 246 7753 CD1 LEU 246 7754 CD2 LEU 246 7755 C LEU 246 7756 O LEU 246 7757 N GLN 247 7758 CA GLN 247 7760 CG GLN 247 7760 CG GLN 247 7761 CD GLN 247 7761 CD GLN 247 7762 OE1 GLN 247 7763 NE2 GLN 247 7766 N TYR 248 7767 CA TYR 248 7768 CB TYR 248 7769 CG TYR 248	72. 958 72. 647 41. 355 1. 00 19. 81 74. 861 73. 785 41. 702 1. 00 15. 52 74. 381 74. 958 40. 986 1. 00 11. 95 75. 157 76. 196 41. 425 1. 00 11. 90 76. 473 76. 162 40. 915 1. 00 17. 74 74. 459 74. 821 39. 470 1. 00 9. 32 73. 883 75. 625 38. 752 1. 00 10. 56 75. 167 73. 819 38. 968 1. 00 8. 50 75. 252 73. 647 37. 518 1. 00 8. 56 76. 481 72. 812 37. 145 1. 00 8. 57 76. 770 72. 639 35. 644 1. 00 11. 81 77. 074 73. 984 35. 008 1. 00 5. 99 77. 949 71. 694 35. 449 1. 00 10. 70 73. 971 72. 944 37. 070 1. 00 10. 18 73. 772 71. 758 37. 349 1. 00 9. 30 73. 994 73. 685 36. 393 1. 00 12. 01 71. 815 73. 144 35. 938 1. 00 12. 01 70. 995 74. 230 35.	B O N B C C B B C C C C C B B B C C C C C C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	7769 CG TYR 248 7770 CD1 TYR 248 7771 CE1 TYR 248 7772 CD2 TYR 248 7773 CE2 TYR 248 7774 CZ TYR 248 7775 OH TYR 248 7776 C TYR 248 7777 O TYR 248 7777 O TYR 248 7777 N PRO 249 7779 CD PRO 249 7780 CA PRO 249	71. 562 71. 727 31. 155 1. 00 11. 76 70. 967 72. 942 31. 498 1. 00 10. 54 69. 689 73. 265 31. 055 1. 00 11. 01 70. 842 70. 843 30. 360 1. 00 9. 97 69. 562 71. 155 29. 911 1. 00 11. 67 68. 989 72. 366 30. 259 1. 00 11. 89 67. 722 72. 674 29. 801 1. 00 10. 14 74. 385 70. 340 33. 353 1. 00 14. 77 75. 384 71. 049 33. 419 1. 00 15. 30 74. 441 69. 014 33. 544 1. 00 15. 88 73. 350 68. 031 33. 636 1. 00 15. 23 75. 739 68. 381 33. 793 1. 00 16. 47	B C B C B C B C B C B C B C B C B C B C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	7781 CB PRO 249 7782 CG PRO 249 7783 C PRO 249 7784 O PRO 249 7785 N LYS 250 7786 CA LYS 250 7787 CB LYS 250 7788 CG LYS 250 7789 CD LYS 250 7790 CE LYS 250	75. 360 66. 947 34. 161 1. 00 16. 57 74. 086 66. 732 33. 417 1. 00 15. 37 76. 568 68. 468 32. 515 1. 00 16. 66 76. 016 68. 446 31. 419 1. 00 15. 91 77. 884 68. 586 32. 647 1. 00 16. 70 78. 721 68. 683 31. 463 1. 00 18. 05 79. 920 69. 591 31. 719 1. 00 17. 36 80. 912 69. 015 32. 681 1. 00 22. 33 82. 204 69. 826 32. 691 1. 00 28. 25 82. 952 69. 757 31. 355 1. 00 26. 52	B C B C B O B N B C B C B C B C B C B C B C

					(Continued)
				FIG. 4-160	,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	7791 7792 7793 7794 7795 7796 7797 7798 7799 7800 7801 7802 7803 7804 7805 7806 7807 7808 7809 7810 7811 7812	NZ LYS C LYS O LYS N THR CA THR CB THR CG2 THR CG2 THR O THR N VAL CA VAL CB VAL CG1 VAL CG2 VAL CG2 VAL CG VAL CG VAL CG VAL CG CG ARG CC ARG CC ARG CC ARG	250 250 250 251 251 251 251 251 252 252 252 252 252	84. 262 70. 465 31. 442 1. 00 26. 19 B 79. 215 67. 313 31. 040 1. 00 17. 64 B 79. 348 66. 409 31. 867 1. 00 20. 20 B 79. 478 67. 160 29. 750 1. 00 15. 06 B 79. 978 65. 905 29. 234 1. 00 14. 91 B 79. 317 65. 537 27. 896 1. 00 13. 86 B 77. 965 65. 144 28. 128 1. 00 14. 97 B 80. 058 64. 389 27. 227 1. 00 13. 23 B 81. 473 66. 016 29. 015 1. 00 15. 66 B 81. 934 66. 831 28. 227 1. 00 18. 88 B 82. 231 65. 194 29. 720 1. 00 15. 28 B 83. 675 65. 195 29. 578 1. 00 15. 13 B 84. 335 64. 717 30. 882 1. 00 15. 13 B 84. 012 65. 701 31. 991 1. 00 11. 83 B 84. 027 64. 264 28. 422 1. 00 17. 21 B 84. 929 <	O N C C C C
MOTA	7811	CG ARG	253	83. 399 64. 137 24. 755 1. 00 26. 72 B 82. 847 64. 920 23. 578 1. 00 28. 87 B 82. 176 66. 132 24. 033 1. 00 36. 20 B 80. 870 66. 221 24. 278 1. 00 38. 47 B 80. 084 65. 164 24. 099 1. 00 39. 84 B 80. 352 67. 360 24. 727 1. 00 37. 97 B 86. 863 63. 863 26. 389 1. 00 19. 71 B 87. 520 64. 886 26. 246 1. 00 21. 87 B 87. 404 62. 656 26. 538 1. 00 18. 34 B 88. 847 62. 434 26. 594 1. 00 15. 15 B	C C N C N C O N C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	7821 7822 7823 7824 7825 7826 7827 7828 7829 7830 7831 7832 7833 7834 7835 7836	CB VAL CG1 VAL C VAL O VAL N PRO CD PRO CA PRO CB PRO CG PRO C PRO O PRO N TYR CA TYR CB TYR CG TYR	254 254 254 254 255 255 255 255 256 256 256	89. 257 61. 924 27. 994 1. 00 16. 16 B 90. 771 61. 759 28. 081 1. 00 15. 18 B 88. 736 62. 868 29. 065 1. 00 16. 46 B 89. 313 61. 397 25. 585 1. 00 14. 67 B 88. 806 60. 272 25. 566 1. 00 14. 87 B 90. 281 61. 757 24. 726 1. 00 13. 62 B 90. 872 63. 081 24. 472 1. 00 12. 90 B 90. 760 60. 777 23. 746 1. 00 12. 62 B 91. 786 61. 566 22. 933 1. 00 11. 40 B 91. 263 62. 969 23. 013 1. 00 11. 65 B 91. 379 59. 645 24. 553 1. 00 12. 46 B 92. 355 59. 831 25. 282 1. 00 13. 25 B 90. 796 58. 469 24. 414 1. 00 12. 53 B 90. 319 57. 205 26. 398 1. 00 12. 42 B 90. 608 56. 082 27. 360 1. 00 14. 53 B	C C C C C C C C C C C C C C C C C C C
ATOM ATOM ATOM	7837 7838 7839	CD1 TYR CE1 TYR CD2 TYR	256 256 256	91. 021 56. 355 28. 662 1. 00 16. 44 B 91. 192 55. 337 29. 596 1. 00 17. 38 B 90. 382 54. 752 27. 010 1. 00 15. 31 B	С

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					FIG. 4-161	(Continued)
ATTOM	g0.40	(ID)) mire	0.5.0	00.510.50.50.	
ATOM	7840		TYR	256	90. 548 53. 724 27. 941 1. 00 16. 91 B	
ATOM ATOM	7841 7842	CZ OH	TYR TYR	256 256	90. 949 54. 030 29. 232 1. 00 16. 54 B 91. 068 53. 042 30. 176 1. 00 17. 03 B	
ATOM	7843		TYR	256		
ATOM	7844		TYR	256	91. 040 56. 094 24. 263 1. 00 11. 63 B 89. 923 55. 765 23. 870 1. 00 13. 76 B	
ATOM	7845		PRO	257	92.141 55.415 23.924 1.00 10.78 B	
ATOM	7846		PRO	257	93. 535 55. 786 24. 231 1. 00 9. 21 B	
ATOM	7847	CA	PRO	257	92.098 54.229 23.068 1.00 9.97 B	
ATOM	7848		PRO	257	93. 473 54. 233 22. 438 1. 00 8. 95 B	
ATOM	7849		PRO	257	94. 326 54. 657 23. 606 1. 00 8. 91 B	
ATOM	7850		PRO	257	91.859 52.949 23.869 1.00 11.12 B	
ATOM	7851	0	PR0	257	92. 694 52. 556 24. 681 1. 00 9. 90 B	
ATOM	7852	N	LYS	258	90.723 52.300 23.648 1.00 11.97 B	
ATOM	7853	CA	LYS	258	90. 444 51. 057 24. 353 1. 00 13. 52 B	
ATOM	7854	CB	LYS	258	88. 930 50. 855 24. 492 1. 00 15. 66 B	
ATOM	7855	CG	LYS	258	88. 305 51. 808 25. 522 1. 00 14. 41 B	C
ATOM	7856	CD	LYS	258	86. 801 51. 730 25. 552 1. 00 18. 08 B	C
ATOM	7857	CE	LYS	258	86. 204 52. 655 26. 627 1. 00 19. 12 B	C
ATOM	7858	NZ	LYS	258	86. 355 52. 156 28. 030 1. 00 14. 62 B	N
ATOM	7859	C	LYS	258	91.101 49.934 23.571 1.00 14.64 B	C
ATOM ATOM	7860 7861	O N	LYS	258	91. 522 50. 139 22. 437 1. 00 16. 07 B	0
ATOM	7862	CA	ALA ALA	259 259	91. 227 48. 760 24. 178 1. 00 16. 22 B	N
ATOM	7863	CB	ALA	259	91. 874 47. 627 23. 515 1. 00 14. 83 B 91. 564 46. 356 24. 261 1. 00 14. 32 B	C
ATOM	7864	CD	ALA	259	A. 1-A	C
ATOM	7865	ŏ	ALA	259	91. 476 47. 476 22. 045 1. 00 16. 09 B 90. 293 47. 415 21. 710 1. 00 15. 64 B	C
ATOM	7866	Ň	GLY	260	92. 477 47. 428 21. 172 1. 00 15. 04 B	O N
ATOM	7867	CA	GLY	260	92. 221 47. 269 19. 754 1. 00 15. 99 B	C
ATOM	7868	C	GLY	260	91. 841 48. 523 18. 982 1. 00 17. 08 B	C
ATOM	7869	0	GLY	260	91. 781 48. 488 17. 752 1. 00 18. 87 B	ŏ
ATOM	7870	N	ALA	261	91.587 49.629 19.673 1.00 14.62 B	N
ATOM	7871	CA	ALA	261	91.198 50.851 18.983 1.00 14.89 B	Ċ
ATOM	7872	CB	ALA	261	90. 557 51. 830 19. 963 1. 00 13. 58 B	č
ATOM	7873	C	ALA	261	92. 379 51. 509 18. 292 1. 00 17. 12 B	C
ATOM	7874	0	ALA	261	93. 489 50. 986 18. 298 1. 00 20. 05 B	0
ATOM	7875	N	VAL	262	92. 135 52. 662 17. 686 1. 00 17. 34 B	N
ATOM	7876		VAL	262	93. 192 53. 384 17. 004 1. 00 16. 00 B	C
ATOM	7877	CB	VAL	262	92.614 54.371 15.947 1.00 14.51 B	С
ATOM	7878		VAL	262	93. 717 55. 252 15. 383 1. 00 13. 59 B	С
ATOM	7879		VAL	262	91. 970 53. 596 14. 820 1. 00 10. 82 B	C
ATOM ATOM	7880 7881	C	VAL VAL	262	93. 984 54. 150 18. 055 1. 00 17. 31 B	C
ATOM	7882	0 N	ASN	262 263	93. 432 54. 973 18. 786 1. 00 20. 51 B	0
ATOM	7883		ASN	263 263	95. 275 53. 856 18. 128 1. 00 16. 87 B 96. 190 54. 493 19. 068 1. 00 17. 45 B	N
ATOM	7884		ASN	263		C
ATOM	7885		ASN	263		C
ATOM	7886	0D1		263	97. 230 52. 629 20. 437 1. 00 20. 08 B 97. 919 51. 606 20. 500 1. 00 19. 88 B	C
ATOM	7887	ND2		263	96. 329 52. 950 21. 365 1. 00 18. 44 B	0 N
ATOM	7888		ASN	263	96. 706 55. 827 18. 533 1. 00 18. 01 B	N C
		-			00.000 00.021 10.000 1.00 10.01 , D	U

					FIO	G. 4-	162			(Continued)
ATOM	7889	0	ASN	263	96. 578	56. 134	17. 345	1.00 19.39	В	0
ATOM	7890	N	PRO	264	97. 288	56.646	19.413	1.00 17.06	В	N
ATOM	7891	CD	PRO	264	97. 357	56.546	20.883	1.00 15.68	В	C
ATOM	7892	CA	PRO	264	97. 819	57. 926	18.950	1.00 15.10	В	C
ATOM	7893	CB	PRO	264	98. 089	58.676	20. 251	1.00 14.78	В	С
ATOM	7894	CG	PRO	264	98.411	57.569	21.214	1.00 14.94	В	C
ATOM	7895	C	PRO	264	99. 105	57.605	18. 198	1.00 15.50	В	С
ATOM	7896	0	PRO	264	99.669	56. 527	18.369	1.00 15.27	В	0
ATOM	7897	N	THR	265	99. 560	58. 521	17. 354	1.00 16.21	В	N
ATOM	7898	CA	THR	265	100. 796	58. 305	16.617	1.00 15.30	В	C
ATOM	7899	CB	THR	265	100.647	58. 677	15. 132	1.00 15.20	В	C
ATOM	7900		THR	265	100.081	59.983	15.029	1.00 17.05	В	0
ATOM	7901		THR	265	99. 747	57. 687	14.415	1.00 10.60	В	C
ATOM ATOM	7902 7903	C	THR THR	265 265	101. 818 101. 454	59. 211 60. 126	17. 279	1.00 16.13	В	C
ATOM	7904	O N	VAL	266	101. 454	58. 971	18. 007 17. 030	1.00 16.83 1.00 17.64	B B	0 N
ATOM	7905	CA	VAL	266	103. 033	59. 781	17.667	1.00 17.04	В	N C
ATOM	7906	CB	VAL	266	104. 116	59.060	18. 930	1.00 17.49	В	C
ATOM	7907		VAL	266	105. 224	57.714	18.538	1.00 13.28	B	Č
ATOM	7908		VAL	266	105. 642	59. 921	19.666	1.00 12.10	В	Č
ATOM	7909	C	VAL	266	105. 312	60.112	16.769	1.00 19.23	B	č
ATOM	7910	Ŏ	VAL	266	105. 693	59. 331	15.893	1.00 18.24	В	ŏ
ATOM	7911	N	LYS	267	105.889	61.287	17.003	1.00 20.19	B	Ň
ATOM	7912	CA	LYS	267	107.058	61.756	16.272	1.00 19.42	B	Ċ
ATOM	7913	CB	LYS	267	106.678	62.855	15. 291	1.00 19.76	B	Č
ATOM	7914	CG	LYS	267	105.786	62.413	14.168	1.00 21.59	В	C
ATOM	7915	CD	LYS	267	105.452	63.605	13. 291	1.00 23.15	В	C
ATOM	7916	CE	LYS	267	104. 593	63.205	12.119	1.00 23.47	В	C
ATOM	7917	NZ	LYS	267	104. 225	64.402	11.334	1.00 27.20	В	N
ATOM	7918	C	LYS	267	108. 032	62.334	17. 288	1.00 19.59	В	C
ATOM	7919	0	LYS	267	107.618	62.826	18.336	1.00 20.86	В	0
ATOM	7920	N	PHE	268	109. 322	62.275	16.984	1.00 19.32	В	N
ATOM	7921	CA	PHE	268	110. 325	62.818	17. 882	1.00 18.94	. В	C
ATOM	7922	CB	PHE	268	111.350	61.757	18. 259	1.00 17.47	В	C
ATOM	7923	CG	PHE	268	112. 186	62.131	19. 444	1.00 16.21	В	C
ATOM	7924		PHE	268	111.601	62. 290	20.692	1.00 16.98	В	C
ATOM	7925		PHE	268	113. 555	62.327	19. 313	1.00 16.35	В	C
ATOM ATOM	7926 7927		PHE PHE	268 268	112. 368 114. 332	62.639	21. 797	1.00 18.80	В	C
ATOM	7928	CZ	PHE	268	113. 737	62. 674 62. 832	20. 405	1.00 17.68	В	C
ATOM	7929	C	PHE	268	111.016	63. 979	21. 655 17. 192	1.00 18.66 1.00 20.34	B B	C C
ATOM	7930	Ö	PHE	268	111.010	64.016	15. 968	1.00 20.34	В	ι 0
ATOM	7931	N	PHE	269	111. 491	64. 931	17. 981	1.00 21.73	В	N N
ATOM	7932	CA	PHE	269	112. 152	66. 105	17. 435	1.00 20.70	В	C
ATOM	7933	CB	PHE	269	111. 141	67. 239	17. 222	1.00 20.14	В	Č
ATOM	7934		PHE	269	110.070	66. 937	16. 216	1.00 21.88	В	Č
ATOM	7935	CD1		269	110.332	67.019	14.853	1.00 22.75	В	Č
ATOM	7936	CD2		269	108. 785	66.605	16.631	1.00 23.20	B	č
ATOM	7937	CE1		269	109. 326	66. 781	13. 912	1.00 21.98	B	č

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	(Continued)							
ATOM 77 ATOM 78 ATOM 79	940 C 941 O 942 N 943 CA 944 CB 944 CG 945 CG2 946 CG2 947 C 948 N 950 CA 951 CB 952 CG1 955 CG 955 CA 956 CA 957 CA 966 OD1 A 967 CA 966 CB 967 CA 968 CG 968 CG 968 CG 969 OD1 A 967 CA 968 CG 970 N 960 OD1 A 967 CA 967 CA 968 CG 971 CA 968 CG 971 CA 972 CA 973 CB 974 CG 975 OD1 A 977 CA 978 O 977 CA 978 O 977 CA 978 CG 97	PHE 269 PHE 269 PHE 269 PHE 269 PHE 270 VAL 270 VAL 270 VAL 270 VAL 270 VAL 271 VAL 27	107. 771 108. 044 113. 209 113. 127 114. 195 115. 239 116. 527 117. 517 116. 219 115. 495 115. 600 115. 561 115. 794 114. 516 114. 096 114. 769 116. 926 117. 094 117. 706 118. 828 119. 951 121. 179 121. 094 122. 330 118. 347 117. 943 118. 397 117. 938 117. 509 118. 653 116. 510 118. 988 118. 669 120. 239 121. 315 122. 671 123. 019 124. 047 122. 267 121. 277 121. 899 120. 456 121. 096 120. 476 119. 030 118. 580	75. 727 74. 960 77. 516 78. 680 77. 157 78. 139 77. 446 77. 049 76. 363 77. 430 78. 996 80. 058 78. 542 79. 279 78. 462 77. 197 79. 652	15. 700 14. 337 18. 402 19. 613 17. 858 18. 667 18. 635 19. 630 18. 985 16. 880 18. 973 18. 546 19. 363 20. 536 18. 728 19. 383 18. 378 19. 383 19. 031 19. 696 18. 841 19. 972 19. 243 21. 292 21. 959 23. 400 24. 181 23. 403 21. 967 22. 208 21. 698 21. 775 23. 193 24. 117 20. 366 18. 166 21. 775 23. 193 24. 117 20. 366 19. 419 20. 366 19. 419 21. 6948 17. 781 16. 673	1.00 23.06 1.00 22.44 1.00 21.66 1.00 21.27 1.00 23.26 1.00 23.57 1.00 23.57 1.00 23.02 1.00 25.32 1.00 26.00 1.00 26.96 1.00 27.45 1.00 28.95 1.00 27.39 1.00 27.39 1.00 27.39 1.00 27.39 1.00 27.39 1.00 27.39 1.00 27.41 1.00 27.39 1.00 27.41 1.00 27.41 1.00 27.62 1.00 28.35 1.00 30.38 1.00 27.41 1.00 27.43 1.00 27.43 1.00 27.43 1.00 27.43 1.00 27.43 1.00 27.43 1.00 27.43 1.00 30.38 1.00 37.48 1.00 37.48 1.00 37.48 1.00 37.48 1.00 37.48 1.00 37.48 1.00 37.48 1.00 37.48 1.00 37.48 1.00 37.48 1.00 37.48 1.00 37.48 1.00 37.48 1.00 37.48 1.00 37.48	888888888888888888888888888888888888888	(Continued) C C C C C C C C C C C C C C C C C C C
ATOM 798	36 CA LI	EU 276	116.949 8			1.00 40.53	В	С

					FIC	G. 4-	164			(Continued)
ATOM ATOM ATOM ATOM ATOM ATOM	7987 7988 7989 7990 7991 7992	CG CD1 CD2 C	LEU LEU LEU LEU LEU	276 276 276 276 276 276 276	116. 076 116. 002 115. 319 115. 261 116. 914 117. 675	80. 425 78. 958 78. 876 78. 134 82. 229 83. 002	19. 664 20. 097 21. 445 19. 057 18. 140 18. 721	1.00 38.58 1.00 36.34 1.00 35.16 1.00 32.57 1.00 41.99 1.00 41.16	B B B B	C C C C C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM	7993 7994 7995 7996 7997 7998 7999	CA CB OG C O N	SER SER SER SER SER SER	277 277 277 277 277 277 277	116. 029 115. 916 116. 489 116. 268 114. 494 113. 529 114. 378	82. 634 84. 044 84. 277 85. 618 84. 586 83. 856 85. 884	17. 233 16. 863 15. 462 15. 044 16. 902 16. 701 17. 148	1.00 44.02 1.00 46.53 1.00 48.49 1.00 50.90 1.00 46.23 1.00 46.82 1.00 46.94	B B B B B	N C C O C O
ATOM ATOM ATOM ATOM ATOM ATOM ATOM	8000 8001 8002 8003 8004 8005 8006	CB OG C O N CA	SER SER SER SER SER SER SER VAL SVAL	278 278 278 278 278 278 279 279	113. 081 113. 204 113. 617 112. 531 111. 325 113. 419 112. 995	86. 535 87. 899 87. 759 86. 710 86. 829 86. 723 86. 889	17. 202 17. 884 19. 234 15. 794 15. 600 14. 808 13. 428	1.00 47.82 1.00 48.09 1.00 49.14 1.00 48.26 1.00 48.73 1.00 48.48	B B B B B	C C O C O N
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	8007 8008 8009 8010 8011 8012 8013 8014	CG1 CG2 C O N CA	VAL VAL VAL VAL THR THR	279 279 279 279 279 280 280 280	114. 189 113. 709 114. 902 112. 340 111. 130 113. 145 112. 651 113. 719	87. 229 87. 454 88. 464 85. 606 85. 433 84. 708 83. 432 82. 709	12. 514 11. 089 13. 037 12. 941 13. 082 12. 380 11. 872 11. 032	1. 00 49. 95 1. 00 50. 61 1. 00 50. 28 1. 00 48. 52 1. 00 49. 49 1. 00 47. 70 1. 00 46. 64 1. 00 47. 86	B B B B B	C C C O N C C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM	8015 8016	OG1 CG2 C O N CA	THR THR THR THR THR ASN ASN	280 280 280 280 280 281 281	113. 179 114. 946 112. 238 112. 586 111. 499 111. 040 109. 744	81. 479 82. 399 82. 484 82. 677 81. 447 80. 454 79. 815	10. 531 11. 883 12. 992 14. 155 12. 622 13. 581 13. 089	1.00 41.80 1.00 48.07 1.00 47.49 1.00 45.40 1.00 44.24 1.00 45.09 1.00 44.81 1.00 46.08	B B B B B	O C C O N C C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	8022 8023 8024 8025 8026 8027 8028	CG OD1 ND2 C O	ASN 2 ASN 2 ASN 2 ASN 2 ASN 2	281 281 281 281 281 281 282	103. 144 108. 592 108. 351 107. 873 112. 088 112. 874 112. 100 113. 045	80. 786 81. 455 80. 868 79. 379 79. 065 78. 823 77. 773	13. 096 14. 101 11. 984 13. 812 12. 919 15. 019	1.00 48.90 1.00 49.62 1.00 52.14 1.00 43.47 1.00 44.44 1.00 41.76 1.00 38.62	B B B B B	C O N C O N
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	8029 8030 8031 8032 8033 8034 8035	CB C O N CA	ALA SALA SALA SALA SALA SALA SALA SALA	282 282 282 282 283 283 283 283	112. 795 112. 863 111. 797 113. 905 113. 828 114. 867 114. 665	77. 301 76. 619 76. 463 75. 816 74. 672 74. 772 75. 994	16. 792 14. 403 13. 815 14. 231 13. 335 12. 218 11. 495	1. 00 36. 02 1. 00 37. 75 1. 00 37. 34 1. 00 36. 86 1. 00 35. 84 1. 00 37. 70 1. 00 41. 71	B B B B B B	C C O N C C C

(C										
					FIG	. 4 -	165			
ATOM	8036		THR	283		73. 595	11. 265	1.00 37.32	В	C
MOTA	8037	C	THR	283		73. 403	14. 125	1.00 33.58	В	C
ATOM ATOM	8038 8039	O N	THR	283		73. 263	14. 774	1.00 34.31	В	0
ATOM	8040	CA	SER SER	284 284	113. 123 113. 250	72. 482 71. 230	14.073	1.00 32.05	В	N
ATOM	8041	CB	SER	284		70. 893	14. 800 15. 507	1.00 30.43 1.00 28.61	B B	C
ATOM	8042	0G	SER	284		71. 761	16.605	1.00 28.01	В	C 0
ATOM	8043	C	SER	284		70.090	13. 883	1.00 30.34	В	C ·
ATOM	8044	Ö	SER	284		69.865	12.850	1.00 31.22	B	ŏ
ATOM	8045	N	ILE	285		69.367	14. 260	1.00 29.19	B	N
ATOM	8046	CA	ILE	285		68. 241	13.457	1.00 28.80	B	Č
ATOM	8047	CB	ILE	285		68.037	13.546	1.00 29.35	В	C
ATOM	8048		ILE	285		66. 979	12.548	1.00 29.12	. В	С
ATOM	8049		ILE	285		69. 350	13. 250	1.00 30.38	В	C
ATOM	8050	CD1		285		70. 303	14. 428	1.00 34.47	В	С
ATOM	8051	C	ILE	285		66. 996	13.976	1.00 28.14	В	C
ATOM ATOM	8052	0 N	ILE	285		66.694	15. 168	1.00 30.23	В	0
ATOM	8053 8054	N CA	GLN GLN	286 286		66. 278	13.078	1.00 25.84	В	N
ATOM	8055		GLN	286		65. 076 64. 886	13.457	1.00 24.81	В	C
ATOM	8056		GLN	286		63. 547	12.550 12.715	1.00 23.81 1.00 23.29	В	C
ATOM	8057		GLN	286		63. 417	11.868	1.00 23.29	B B	C C
ATOM	8058	0E1		286		52. 388	11.894	1.00 25.38	В	0
ATOM	8059	NE2		286		34. 461	11.110	1.00 23.87	В	N
ATOM	8060		GLN	286		33. 838	13. 386	1.00 25.74	В	Č
ATOM	8061	0	GLN	286		53. 732	12.526	1.00 26.39	B	ŏ
ATOM	8062		ILE	287		52. 908	14.307	1.00 24.54	B	N
ATOM	8063		ILE	287		31.655	14.346	1.00 23.40	В	С
ATOM	8064		ILE	287		61. 481	15. 694	1.00 21.87	В	C
ATOM	8065	CG2		287		50. 143	15. 728	1.00 20.61	В	C
ATOM	8066	CG1		287		632	15.887	1.00 19.27	В	C
ATOM ATOM	8067	CD1		287		52. 506	17.113	1.00 20.58	В	C
ATOM	8068 8069		ILE ILE	287 287		50. 578	14. 186	1.00 24.59	В	C
ATOM	8070		THR	288		60. 204 60. 093	15. 142	1.00 27.03	В	0
ATOM	8071		THR	288			12. 966 12. 708	1.00 25.43	В	N
ATOM	8072		THR	288			11. 188	1.00 26.10 1.00 26.69	B B	C
ATOM	8073		THR	288			10. 539	1.00 26.37	В	0
ATOM	8074	CG2		288				1.00 25.25	В	Č
ATOM	8075		THR	288				1.00 26.85	В	č
ATOM	8076		THR	288				1.00 27.04	B	ŏ
ATOM	8077		ALA	289	111.484 5			1.00 28.37	B	Ň
ATOM	8078		ALA	289			14. 325	1.00 27.90	В	Ċ
ATOM	8079		ALA	289				1.00 26.91	В	Č
ATOM	8080		ALA	289				1.00 27.44	В	С
ATOM			ALA	289				1.00 28.30	В	0
ATOM ATOM			PRO	290				1.00 26.01	В	N
ATOM			PRO PRO	290 290				1.00 24.74	В	C
111 010	000 1	va I	. NV		113.445 5: SUBSTITUTE S			1.00 25.29	В	С

						(Continued)
					FIG. 4-166	(Continued)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	8085 8086 8087 8088 8089 8090 8091 8092 8093	CB CG C O N CA CB C	PRO PRO PRO ALA ALA ALA ALA	290 290 290 290 291 291 291 291	113. 949 51. 587 14. 138 1. 00 25. 76 B 114. 151 52. 467 15. 342 1. 00 25. 10 B 112. 465 51. 931 12. 110 1. 00 25. 85 B 111. 255 51. 961 12. 330 1. 00 25. 95 B 112. 988 51. 345 11. 038 1. 00 25. 39 B 112. 143 50. 730 10. 024 1. 00 26. 17 B 112. 987 50. 271 8. 846 1. 00 26. 28 B 111. 337 49. 568 10. 573 1. 00 27. 18 B 110. 203 49. 331 10. 145 1. 00 27. 46 B	C C C O N C C C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	8094 8095 8096 8097 8098 8099 8100 8101 8102 8103	N CA CB OG C O N CA CB CG	SER SER SER SER SER MET MET MET	292 292 292 292 292 292 293 293 293 293	111. 916 48. 843 11. 521 1. 00 27. 54 B 111. 220 47. 704 12. 103 1. 00 28. 19 B 112. 161 46. 892 12. 993 1. 00 28. 00 B 112. 525 47. 626 14. 145 1. 00 32. 22 B 110. 027 48. 182 12. 922 1. 00 28. 13 B 109. 176 47. 376 13. 307 1. 00 29. 52 B 109. 976 49. 487 13. 190 1. 00 25. 00 B 108. 881 50. 072 13. 955 1. 00 24. 80 B 109. 387 51. 173 14. 892 1. 00 24. 61 B 110. 231 50. 703 16. 060 1. 00 26. 88 B	N C C O C O N C C C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	8104 8105 8106 8107 8108 8109 8110 8111	SD CE C O N CA CB CG	MET MET MET MET LEU LEU LEU LEU	293 293 293 293 294 294 294 294	109. 323 49. 647 17. 189 1. 00 27. 80 B 110. 457 48. 319 17. 438 1. 00 25. 74 B 107. 836 50. 677 13. 027 1. 00 24. 57 B 106. 641 50. 528 13. 252 1. 00 25. 32 B 108. 292 51. 360 11. 983 1. 00 24. 37 B 107. 393 52. 008 11. 041 1. 00 23. 80 B 108. 183 52. 930 10. 114 1. 00 23. 40 B 108. 945 54. 072 10. 786 1. 00 24. 87 B	S C C O N C C C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	8112 8113 8114 8115 8116 8117 8118 8119 8120	CD2 C O N CA CB CG2	LEU LEU LEU ILE ILE ILE ILE ILE	294 294 294 294 295 295 295 295 295	109. 806 54. 787 9. 758 1. 00 22. 08 B 107. 958 55. 037 11. 440 1. 00 23. 08 B 106. 540 51. 059 10. 204 1. 00 23. 95 B 105. 714 51. 510 9. 422 1. 00 25. 36 B 106. 724 49. 754 10. 357 1. 00 23. 92 B 105. 923 48. 812 9. 580 1. 00 25. 26 B 106. 601 47. 444 9. 453 1. 00 26. 06 B 107. 972 47. 595 8. 812 1. 00 26. 54 B 106. 698 46. 796 10. 831 1. 00 24. 44 B	C C O N C C C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	8121 8122 8123 8124 8125 8126 8127 8128 8129 8130	CD1 C O N CA C O N CA CB	ILE ILE GLY GLY GLY GLY ASP ASP ASP	295 295 295 296 296 296 297 297	107. 211 45. 388 10. 789 1. 00 28. 37 B 104. 564 48. 575 10. 221 1. 00 26. 01 B 103. 805 47. 712 9. 775 1. 00 28. 75 B 104. 263 49. 328 11. 273 1. 00 24. 77 B 102. 992 49. 167 11. 951 1. 00 22. 28 B 102. 908 50. 040 13. 182 1. 00 21. 29 B 103. 820 50. 818 13. 447 1. 00 20. 80 B 101. 818 49. 920 13. 935 1. 00 20. 38 B 101. 654 50. 718 15. 141 1. 00 20. 14 B 100. 366 50. 339 15. 874 1. 00 21. 58 B	C C O N C C O N C
ATOM ATOM ATOM	8131 8132 8133		ASP ASP ASP	297 297 297	99. 109 50. 665 15. 078 1. 00 22. 60 B 98. 016 50. 234 15. 502 1. 00 25. 00 B 99. 200 51. 350 14. 041 1. 00 22. 18 B	C 0 0

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				FIG	. 4 -	167			(Conti	nued)
ATOM	8134	C ASP	297	102.845	50. 481	16.065	1.00 20.31	В	C	
ATOM	8135	0 ASP	297	103.419	49.390	16.096	1.00 20.82	В	0	
ATOM	8136	N HIS	298	103. 220	51.508	16.814	1.00 16.87	В	N	
ATOM	8137	CA HIS	298	104.335	51.384	17. 734	1.00 16.48	В	C	
ATOM	8138	CB HIS	298	105.669	51.399	16.968	1.00 14.91	В	Ċ	
ATOM	8139	CG HIS	298	105.868	52. 628	16. 137	1.00 12.24	В	C	
ATOM	8140	CD2 HIS	298	106. 539	53. 775	16. 391	1.00 10.39	В	C	
ATOM	8141	ND1 HIS	298	105. 264	52. 802	14.909	1.00 11.35	В	N	
ATOM	8142	CE1 HIS	298	105. 551	54.005	14. 445	1.00 11.25	В	C	
ATOM	8143	NE2 HIS	298	106. 323	54.616	15. 326	1.00 11.96	В	N	
ATOM	8144	C HIS	298	104. 274	52. 560	18.693	1.00 15.84	В	C	
ATOM	8145	0 HIS	298	103.484	53. 476	18. 505	1.00 17.04	В	0 N	
ATOM ATOM	8146	N TYR	299	105.127	52. 539	19. 706	1.00 15.50	В	N	
ATOM ATOM	8147 8148	CA TYR CB TYR	299 299	105.163 104.640	53. 599 53. 095	20. 698 22. 047	1.00 15.35	B B	C	
ATOM	8149	CG TYR	299	104. 040	52. 320	22. 047	1.00 14.51 1.00 14.30	В	C C	
ATOM	8150	CD1 TYR	299	103. 343	52. 973	21. 942	1.00 14.30	В	Č	
ATOM	8151	CE1 TYR	299		52. 269	22. 019	1.00 15.49	В	C	
ATOM	8152	CD2 TYR	299		50. 933	22. 198	1.00 14.56	В	Č	
ATOM	8153	CE2 TYR	299	102. 150	50. 216		1.00 15.40	В	Č	
ATOM	8154	CZ TYR	299		50. 891	22. 186	1.00 15.73	В	č	
ATOM	8155	OH TYR	299		50. 197	22. 286	1.00 15.37	B	ŏ	
ATOM	8156	C TYR	299		54.084	20.952	1.00 16.54	B	č	
ATOM	8157	0 TYR	299	107. 559	53. 364	20.732	1.00 15.53	В	0	
ATOM	8158	N LEU	300	106.688	55.316	21.428	1.00 16.67	В	N	
ATOM	8159	CA LEU	300		55.853	21.818	1.00 17.75	В	C	
ATOM	8160	CB LEU	300		57.367	21.654	1.00 18.54	В	C	
ATOM	8161	CG LEU	300		58.059	22. 183	1.00 20.06	В	С	
ATOM	8162	CD1 LEU	300		57. 535	21.429	1.00 20.50	В	C	
ATOM	8163	CD2 LEU	300		59. 567	22.024	1.00 20.10	В	C	
ATOM	8164	C LEU	300		55. 477	23. 294	1.00 18.55	В	C	
ATOM ATOM	8165	0 LEU	300		55. 783	23. 935	1.00 20.71	В	0	
ATOM	8166 8167	N CYS CA CYS	301 301		54. 805	23.849	1.00 18.50	В	N	
ATOM	8168	CB CYS	301		54. 418 52. 907	25. 252 25. 375	1.00 20.22	В	C	
ATOM	8169	SG CYS	301		51.905	24. 722	1.00 20.55 1.00 26.11	B B	C S	
ATOM	8170	C CYS	301		54. 842	26. 194	1.00 20.11	В	C	
ATOM	8171	0 CYS	301		54. 579	27. 395	1.00 20.62	В	0	
ATOM	8172	N ASP	302		55. 496	25.662	1.00 21.02	В	N	
ATOM	8173	CA ASP	302		55. 968	26. 481	1.00 20.03	В	C	
ATOM	8174	CB ASP	302		54.810	27. 014	1.00 20.49	В	Č	
ATOM	8175	CG ASP	302		55. 296	27. 868	1.00 25.77	B	č	
ATOM	8176	OD1 ASP	302		55. 344	29. 109	1.00 26.02	B	ŏ	
ATOM	8177	OD2 ASP	302		55.664	27. 297	1.00 27.73	B	Ŏ	
ATOM	8178	C ASP	302		56. 894	25.711	1.00 20.08	B	č	
ATOM	8179	Ò ASP	302	113.367	56. 596	24.586	1.00 19.30	В	Ö	
ATOM	8180	n val	303		58.010	26.343	1.00 20.41	В	N	
ATOM	8181	CA VAL	303		59.000	25.756	1.00 20.36	В	С	
ATOM	8182	CB VAL	303	113.435	60. 316	25.470	1.00 19.97	В	С	

	(Continued)							
ATOM 81 ATOM 82 ATOM 83	84 CG2 1	VAL 303 VAL 303 VAL 303 THR 304 THR 305 TRP 3	114. 387 112. 260 115. 267 114. 950 116. 536 117. 639 118. 008 116. 869 119. 136 118. 925 119. 579 119. 307 120. 545 120. 696 119. 682 119. 834 118. 614 120. 885 118. 414 117. 764 118. 413 120. 689 119. 459 121. 722 121. 743 122. 697 123. 899 124. 350 124. 975 125. 086 126. 894 127. 892 127. 892 126. 894 127. 892 125. 397 124. 177 126. 210 125. 699 126. 762	65. 413 64. 928 64. 232 65. 077 66. 242 65. 746 66. 395 60. 875 60. 552 60. 551 59. 864 58. 969 60. 882 60. 767 61. 885 62. 964 62. 744 62. 855 61. 374 64. 250 64. 326 65. 249 66. 540 67. 634	24. 857 24. 540 26. 788 27. 939 26. 389 27. 332 28. 046 28. 751 29. 026 26. 729 25. 952 27. 102 26. 583 26. 975 26. 354 25. 150 24. 917 24. 243 26. 794 25. 938 23. 812 22. 943 27. 148 28. 338 26. 285 26. 673 27. 000 28. 007 26. 133 27. 000 28. 007 26. 133 27. 000 28. 040 25. 659 25. 812 25. 731 25. 749 25. 022 25. 175	1. 00 20. 23 1. 00 17. 52 1. 00 21. 02 1. 00 19. 39 1. 00 21. 48 1. 00 19. 77 1. 00 19. 55 1. 00 20. 57 1. 00 22. 96 1. 00 25. 30 1. 00 22. 41 1. 00 20. 21 1. 00 18. 79 1. 00 20. 14 1. 00 18. 65 1. 00 17. 49 1. 00 18. 37 1. 00 19. 16 1. 00 19. 59 1. 00 21. 43 1. 00 22. 21 1. 00 21. 31 1. 00 22. 53 1. 00 21. 31 1. 00 20. 65 1. 00 21. 97 1. 00 20. 32 1. 00 23. 85 1. 00 24. 42 1. 00 25. 33 1. 00 25. 33 1. 00 25. 73 1. 00 26. 09 1. 00 24. 49 1. 00 24. 49 1. 00 22. 95 1. 00 21. 20	B B B B B B B B B B B B B B B B B B B	CCCONCCOCCONCCCCCNCCCONCCCONCCCONCCO
ATOM 83 ATOM 83 ATOM 83 ATOM 83 ATOM 83	222 CB 223 CG 224 CD 225 OE1		3 126. 762 3 127. 301 3 126. 256 3 126. 477 3 125. 116	67. 634 67. 811 68. 296 68. 290 68. 727		1.00 22.95 1.00 21.20 1.00 20.30 1.00 23.08 1.00 21.02 1.00 25.09	B B B B B	C C C O N C
ATOM 8: ATOM 8: ATOM 8:	228 O 229 N 230 CA 231 CB	GLN 309 GLU 309 GLU 309	3 124. 612 9 125. 687 9 125. 370	67. 411 65. 459 65. 374	23. 095 22. 855 21. 440 20. 627	1.00 26.23 1.00 25.59 1.00 26.16 1.00 25.99	B B B	0 N C C

•	FIG. 4-169	(Continued)
ATOM 8232 CG GLU ATOM 8233 CD GLU ATOM 8234 OE1 GLU ATOM 8235 OE2 GLU ATOM 8236 C GLU ATOM 8237 O GLU ATOM 8238 N ARG ATOM 8239 CA ARG ATOM 8240 CB ARG ATOM 8241 CG ARG ATOM 8242 CD ARG ATOM 8243 NE ARG ATOM 8244 CZ ARG ATOM 8245 NH1 ARG ATOM 8246 NH2 ARG ATOM 8247 C ARG ATOM 8248 O ARG ATOM 8247 C ARG ATOM 8248 O ILE ATOM 8250 CA ILE ATOM 8251 CB ILE ATOM 8251 CB ILE ATOM 8252 CG2 ILE ATOM 8252 CG2 ILE ATOM 8253 CG1 ILE ATOM 8253 CG1 ILE ATOM 8254 CD1 ILE ATOM 8255 C ILE ATOM 8256 O ILE ATOM 8256 O ILE ATOM 8256 C ILE ATOM 8257 N SER ATOM 8258 CA SER ATOM 8259 CB SER ATOM 8260 OG SER ATOM 8261 C SER ATOM 8260 OG SER ATOM 8261 C SER ATOM 8262 O SER ATOM 8263 N LEU ATOM 8264 CA LEU ATOM 8265 CB LEU ATOM 8265 CB LEU ATOM 8266 CG LEU ATOM 8267 CD1 LEU ATOM 8267 CD1 LEU ATOM 8268 CD2 LEU ATOM 8269 C LEU ATOM 8269 C LEU ATOM 8260 CG LEU ATOM 8260 CG LEU ATOM 8260 CG LEU ATOM 8261 C SER ATOM 8262 C SER ATOM 8263 N LEU ATOM 8264 CA LEU ATOM 8265 CB LEU ATOM 8266 CG LEU ATOM 8267 CD1 LEU ATOM 8267 CD1 LEU ATOM 8268 CD2 LEU ATOM 8269 C LEU ATOM 8260 CG LEU ATOM 8270 O LEU ATOM 8271 N GLN ATOM 8272 CA GLN ATOM 8273 CB GLN ATOM 8273 CB GLN ATOM 8274 CG GLN ATOM 8277 NE2 GLN ATOM 8277 NE2 GLN ATOM 8277 NE2 GLN ATOM 8277 NE2 GLN ATOM 8278 C GLN ATOM 8278 C GLN ATOM 8279 O GLN	FIG. 4 - 169 309	Continued B C B C C B C C B C C C C C C C C C C
ATOM 8280 N TRP	315 111.984 52.372 21.108 1.00 22.35	B N

										(Continued)
					FIC	G. 4-	170			,
ATOM	8281	CA	TRP	315	110.672	52. 262	20. 484	1.00 21.75	В	С
ATOM	8282	CB	TRP	315	110.769	52.440	18.968	1.00 21.09	В	С
ATOM	8283	CG	TRP	315	111.376	53. 741	18.540	1.00 21.09	В	C
ATOM	8284	CD2		315	110.678	54.940	18.176	1.00 19.81	В	С
ATOM	8285	CE2		315	111.654	55.901	17.824	1.00 20.24	В	C C
ATOM	8286	CE3		315	109. 325	55. 295	18.113	1.00 17.16	В	C
ATOM	8287	CD1		315	112. 705	54.018	18.405	1.00 21.12	В	C
ATOM	8288	NE1		315	112. 880	55. 310	17. 974	1.00 21.84	В	N
ATOM	8289	CZ2		315	111. 321	57. 197	17.413	1. 00 18. 97	В	C
ATOM	8290	CZ3		315	108. 992	56. 588	17. 704	1.00 20.13	В	C
ATOM	8291		TRP	315	109. 990	57. 522	17. 359	1.00 19.26	В	C
ATOM	8292	C	TRP	315	110.118	50. 880	20. 790	1.00 22.37	В	C
ATOM	8293	0	TRP	315	110.877	49. 922	20. 941	1.00 24.80	В	0 N
ATOM	8294	N	LEU	316	108.799	50. 772	20. 872 21. 184	1.00 21.02 1.00 20.90	B B	N
ATOM ATOM	8295 8296	CA CB	LEU LEU	316 316	108. 159 107. 653	49. 502 49. 544	21. 104 22. 628	1.00 20.90	В	C C
ATOM	8297	CG	LEU	316	106.866	48. 358	23. 194	1.00 19.46	В	C
ATOM	8298		LEU	316	107. 786	47. 157	23. 408	1.00 13.40	В	Č
ATOM	8299		LEU	316	106. 223	48. 783	24. 501	1.00 16.22	В	č
ATOM	8300		LEU	316	106. 995	49. 228	20. 229	1.00 20.90	В	č
ATOM	8301	ŏ .	LEU	316	106.161	50.098	20. 000	1.00 22.41	B	ŏ
ATOM	8302	Ň	ARG	317	106. 941	48. 026	19.666	1.00 19.89	B	N
ATOM	8303	CA	ARG	317	105.851	47.678	18.753	1.00 20.30	В	Ċ
ATOM	8304	CB	ARG	317	106. 154	46. 362·	18.035	1.00 20.73	В	Ċ
ATOM	8305	CG	ARG	317	107. 248	46.480	16.993	1.00 23.49	В	C
ATOM	8306	CD	ARG	317	107. 524	45.149	16.321	1.00 24.95	В	C
ATOM	8307	NE	ARG	317	108. 347	45.314	15. 128	1.00 25.57	В	N
ATOM	8308	CZ	ARG	317	108.925	44. 313	14. 476	1.00 26.73	В	C
ATOM	8309	NH1		317	108.775	43.061	14.897	1.00 23.81	В	N
ATOM	8310	NH2		317	109.656	44.567	13. 401	1.00 29.12	В	N
ATOM	8311	C	ARG	317	104. 537	47. 545	19. 512	1.00 19.31	В	C
ATOM	8312	0	ARG	317	104. 541	47. 266	20. 713	1.00 17.59	В	0
ATOM	8313	N	ARG	318	103. 415	47. 747	18. 820	1.00 18.54	В	N
ATOM	8314	CA	ARG	318	102.117	47. 621	19.476	1.00 17.04	В	C
ATOM	8315	CB	ARG	318	100.970	47. 781	18. 483	1.00 17.09	В	C
ATOM	8316	CG	ARG	318	99.608	47. 794	19. 164	1.00 17.74	В	C
ATOM	8317	CD	ARG	318	98. 613	48.660	18. 414	1.00 16.48	В	C .
ATOM	8318	NE CZ	ARG	318 318	97. 326 96. 320	48. 672 49. 478	19. 092 18. 771	1.00 16.05 1.00 17.02	В	N C
ATOM ATOM	8319 8320		ARG ARG	318	96. 464	50.342	17. 771	1.00 17.02	B B	N N
ATOM	8321		ARG	318	95. 180	49. 428	19. 460	1.00 13.39	B	N N
ATOM	8322	C	ARG	318	102. 085	46. 251	20. 132	1.00 12.42	B	C
ATOM	8323	Ŏ	ARG	318	101.569	46. 103	21. 234	1.00 15.26	В	0
ATOM	8324	N	ILE	319	102.627	45. 251	19. 440	1.00 15.14	В	N
ATOM	8325	CA	ILE	319	102. 757	43. 912	20.007	1.00 15.27	В	Č
ATOM	8326	CB	ILE	319	103.006	42.848	18. 949	1.00 15.60	B	č
ATOM	8327		ILE	319	103. 268	41.519	19.621	1.00 17.64	B	č
ATOM	8328		ILE	319	101. 793	42. 732	18.036	1.00 15.37	B	č
ATOM	8329		ILE	319	100.524	42.425	18. 781	1.00 15.54	В	Ċ

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				FIG. 4-171	(Continued)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	8330 8331 8332 8333 8334 8335 8336 8337 8340 8341 8342 8343 8344	C ILE O ILE N GLN CA GLN CB GLN CD GLN OE1 GLN NE2 GLN C GLN O GLN N ASN CA ASN CB ASN CG ASN OD1 ASN	319 320 320 320 320 320 320 320 321 321 321 321	104.036 44.122 20.802 1.00 16.78 B 105.145 44.086 20.257 1.00 16.37 B 103.850 44.367 22.092 1.00 17.82 B 104.923 44.693 23.016 1.00 18.01 B 104.293 45.341 24.248 1.00 16.84 B 103.383 46.495 23.863 1.00 16.48 B 102.833 47.250 25.048 1.00 17.06 B 103.544 47.509 26.016 1.00 18.02 B 101.566 47.633 24.966 1.00 16.46 B 105.964 43.663 23.437 1.00 18.97 B 106.399 43.654 24.594 1.00 20.18 B 106.382 42.800 22.520 1.00 19.64 B 107.420 41.846 22.875 1.00 21.44 B 106.409 40.085 21.332 1.00 27.68 B 106.593 40.839 20.374 1.00 28.16 B	C O N C C C O N C C C C O O C C C O
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	8345 8346 8347 8348 8350 8351 8352 8353 8354 8355 8356 8357 8358 8359 8360 8361	ND2 ASN C ASN O ASN N TYR CA TYR CB TYR CC TYR CCI TYR CI TYR C	321 321 321 322 322 322 322 322 322 322	106. 593 40. 839 20. 374 1.00 28. 16 B 105. 745 38. 934 21. 255 1.00 30. 91 B 108. 658 42. 087 22. 036 1.00 21. 63 B 109. 533 41. 228 21. 940 1.00 23. 87 B 108. 735 43. 275 21. 444 1.00 20. 56 B 109. 873 43. 644 20. 613 1.00 18. 63 B 109. 605 43. 208 19. 178 1.00 18. 95 B 110. 766 43. 362 18. 228 1.00 21. 29 B 111. 086 44. 604 17. 677 1.00 21. 18 B 112. 118 44. 733 16. 759 1.00 22. 17 B 111. 520 42. 252 17. 840 1.00 20. 55 B 112. 557 42. 372 16. 925 1.00 21. 33 B 112. 847 43. 611 16. 387 1.00 22. 88 B 113. 855 43. 726 15. 461 1.00 28. 00 B 110. 115 45. 149 20. 678 1.00 18. 95 B 109. 240	0 N C C C C C C C C C O N
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	8362 8363 8364 8365 8366 8367 8368 8369 8370 8371 8372 8373 8374 8375 8376 8377 8378	CA SER CB SER OG SER C SER O SER N VAL CA VAL CB VAL CG1 VAL CG2 VAL C VAL O VAL N MET CA MET CB MET CG MET SD MET	323 323 323 323 324 324 324 324 324 325 325 325 325 325	111. 657 46. 946 21. 233 1. 00 17. 89 B 111. 623 47. 418 22. 684 1. 00 18. 88 B 112. 602 46. 740 23. 444 1. 00 21. 21 B 113. 057 47. 131 20. 677 1. 00 16. 99 B 113. 851 46. 190 20. 657 1. 00 15. 79 B 113. 360 48. 345 20. 230 1. 00 16. 51 B 114. 672 48. 638 19. 664 1. 00 17. 39 B 114. 612 48. 684 18. 126 1. 00 18. 70 B 113. 454 49. 550 17. 692 1. 00 22. 04 B 115. 901 49. 257 17. 565 1. 00 20. 08 B 115. 201 49. 970 20. 151 1. 00 16. 54 B 114. 460 50. 946 20. 243 1. 00 19. 05 B 116. 487 50. 011 20. 463 1. 00 15. 89 B 117. 104 51. 243 20. 914 1. 00 16. 61 B 118. 682 52. 280 22. 597 1. 00 19. 56 B 119.	CCCCCCNCCCS

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					(Continued)
	•			FIG. 4-173	(Continued)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	8428 8429 8430 8431 8432 8433 8434 8435 8436 8437 8438 8444 8445 8445 8445 8445 8453 8453	OD2 ASP C ASP O ASP N GLU CB GLU CB GLU CC GLU OE1 GLU OE2 GLU OE2 GLU OE3 SER CA GLY CA GLY CA ARG	331 331 332 332 332 332 332 332 332 333 333	126. 387 65. 018 9. 543 1. 00 41. 37 B 127. 770 65. 966 10. 967 1. 00 40. 07 B 126. 355 67. 395 13. 062 1. 00 41. 15 B 125. 641 68. 126 12. 380 1. 00 40. 39 B 127. 358 67. 852 13. 802 1. 00 44. 16 B 127. 690 69. 271 13. 879 1. 00 47. 17 B 129. 001 69. 457 14. 646 1. 00 48. 80 B 129. 367 70. 901 14. 922 1. 00 51. 70 B 130. 451 71. 028 15. 979 1. 00 54. 56 B 130. 203 70. 623 17. 136 1. 00 55. 51 B 131. 552 71. 528 15. 658 1. 00 56. 11 B 127. 791 69. 941 12. 517 1. 00 47. 83 B 128. 179 69. 175 11. 505 1. 00 48. 69 B 128. 312 69. 715 10. 161 1. 00 <td>0 C O N C C C C O C O N C C O C O N C C O C O</td>	0 C O N C C C C O C O N C C O C O N C C O C O
ATOM ATOM	8462 8463	NE ARG CZ ARG	336 336 336	119. 339 66. 597 8. 248 1. 00 45. 61 B 118. 019 67. 002 8. 729 1. 00 48. 18 B 117. 522 68. 233 8. 613 1. 00 49. 86 B	
ATOM ATOM ATOM ATOM	8464 8465 8466 8467	NH1 ARG NH2 ARG C ARG O ARG	336 336 336 336	118. 229 69. 194 8. 025 1. 00 50. 51 B 116. 317 68. 510 9. 094 1. 00 50. 56 B 121. 524 65. 817 12. 654 1. 00 35. 64 B 122. 629 65. 900 13. 181 1. 00 35. 91 B	N N C
ATOM ATOM ATOM ATOM	8468 8469 8470 8471	N TRP CA TRP CB TRP CG TRP	337 337 337	120.649 64.865 12.955 1.00 33.09 B 120.955 63.818 13.918 1.00 30.08 B 119.922 63.793 15.053 1.00 24.67 B	O N C C C C
ATOM ATOM ATOM	8472 8473 8474	CD2 TRP CE2 TRP CE3 TRP	337 337 337 337	119.993 64.979 15.954 1.00 20.03 B 120.670 65.059 17.214 1.00 17.75 B 120.550 66.390 17.671 1.00 17.16 B 121.374 64.137 17.997 1.00 15.36 B	C C
ATOM ATOM	8475 8476	CD1 TRP NE1 TRP	337 337	119. 498 66. 224 15. 709 1. 00 19. 73 B 119. 827 67. 079 16. 736 1. 00 18. 61 B	C N

		FIG. 4-1	174	(Continued)
ATOM 8513 ATOM 8514 ATOM 8515 ATOM 8516 ATOM 8517	CZ3 TRP CH2 TRP C TRP O TRP N ASN CA ASN CB ASN CB ASN OD1 ASN ND2 ASN C ASSN C CYS	337	18. 875 1. 00 18. 08 B 19. 196 1. 00 15. 24 B 19. 622 1. 00 16. 71 B 13. 188 1. 00 31. 57 B 12. 482 1. 00 32. 12 B 12. 691 1. 00 32. 12 B 12. 691 1. 00 34. 88 B 10. 471 1. 00 38. 68 B 10. 251 1. 00 39. 82 B 9. 669 1. 00 33. 60 B 13. 499 1. 00 33. 60 B 14. 385 1. 00 34. 06 B 3. 564 1. 00 34. 06 B 4. 961 1. 00 37. 83 B 5. 160 1. 00 37. 83 B 3. 665 1. 00 32. 80 B 2. 933 1. 00 34. 61 B 2. 609 1. 00 34. 61 B 2. 609 1. 00 34. 95 B 4. 418 1. 00 34. 95 B	CCCCONCCONCONCCOCSNCCCCCONCCCCONCCCONCC
	CA ARG CB ARG CC ARG CD ARG NE ARG CZ ARG NH1 ARG NH2 ARG	343 124. 303 51. 074 1 343 124. 611 52. 562 1 343 126. 063 52. 922 1 343 126. 345 54. 396 1 343 127. 775 54. 692 1 343 128. 301 55. 885 1 343 127. 516 56. 907 1 343 129. 615 56. 052 1		

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					(Continued)
				FIG. 4-175	(Constituca)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	8526 8527 8528 8529 8530 8531 8532 8534 8535 8536 8537 8538 8539 8540 8541	O ARG N. GLN CA GLN CB GLN CD GLN OE1 GLN NE2 GLN O GLN N HIS CA HIS CB HIS CCH HIS CD	343 344 344 344 344 344 345 345 345 345	122. 586 51. 143 18. 650 1. 00 28. 30 B 122. 121 50. 026 16. 763 1. 00 28. 05 B 120. 786 49. 625 17. 183 1. 00 28. 26 B 119. 944 49. 238 15. 974 1. 00 26. 68 B 118. 980 50. 296 15. 516 1. 00 30. 39 B 118. 091 49. 802 14. 399 1. 00 31. 50 B 117. 567 48. 685 14. 457 1. 00 31. 52 B 117. 905 50. 632 13. 378 1. 00 32. 84 B 120. 853 48. 431 18. 121 1. 00 28. 55 B 121. 655 47. 515 17. 919 1. 00 28. 32 B 120. 008 48. 436 19. 145 1. 00 28. 34 B 120. 514 47. 753 21. 452 1. 00 28. 88 B 121. 973 48. 079 21. 443 1. 00 27. 88 B 123. 062 47. 279 21. 516 1. 00 <td>(Continued) 0 N C C C C O N C C C O N C C C C O N C C C C</td>	(Continued) 0 N C C C C O N C C C O N C C C C O N C C C C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	8543 8544 8545 8546 8547 8548 8550 8551 8552 8553 8554 8555 8556	NE2 HIS C HIS O HIS N ILE CA ILE CB ILE CG2 ILE CG1 ILE CD1 ILE C ILE O ILE N GLU CA GLU CB GLU	345 345 346 346 346 346 346 346 347 347	124.166 48.086 21.381 1.00 28.63 B 118.568 46.799 20.215 1.00 27.76 B 117.659 47.508 20.625 1.00 30.01 B 118.396 45.538 19.849 1.00 26.83 B 117.102 44.897 19.899 1.00 25.72 B 116.977 43.842 18.791 1.00 25.56 B 115.655 43.114 18.919 1.00 26.17 B 117.102 44.517 17.422 1.00 26.62 B 117.180 43.544 16.263 1.00 26.42 B 116.854 44.218 21.228 1.00 26.11 B 117.736 43.558 21.776 1.00 25.75 B 115.645 44.396 21.746 1.00 26.23 B 115.260 43.767 22.994 1.00 25.82 B 115.226 44.777 24.134 1.00 25.51 B <td>N C C C C C C C C C C C C C C C C C C C</td>	N C C C C C C C C C C C C C C C C C C C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	8557 8558 8559 8560 8561 8562 8563 8564 8565 8566 8567 8568 8569 8570 8571 8572 8573 8574	CG GLU OE1 GLU OE2 GLU O GLU O GLU N MET CA MET CB MET CB MET CC MET O M	347 347 347 347 347 348 348 348 348 348 348 349 349 349	115. 282 44. 118 25. 505 1. 00 28. 20 B 115. 107 45. 094 26. 652 1. 00 29. 16 B 115. 667 46. 208 26. 592 1. 00 29. 18 B 114. 415 44. 736 27. 628 1. 00 32. 76 B 113. 873 43. 172 22. 799 1. 00 26. 44 B 112. 919 43. 889 22. 495 1. 00 26. 00 B 113. 770 41. 858 22. 957 1. 00 26. 58 B 112. 492 41. 181 22. 807 1. 00 27. 90 B 112. 270 40. 767 21. 345 1. 00 30. 41 B 113. 466 40. 132 20. 660 1. 00 34. 65 B 113. 695 38. 420 21. 117 1. 00 42. 21 B 112. 371 39. 980 23. 732 1. 00 26. 60 B 113. 363 39. 472 24. 247 1. 00 26. 08 B 11. 135 39. 549 23. 950 1. 00 <td>C C C C C C C C C C C C C C C C C C C</td>	C C C C C C C C C C C C C C C C C C C

					FIC	G. 4 -	176			(Cont	inued)
ATOM	8575	С	SER	349	110.084	37. 387	24. 005	1.00 21.88	В	С	
ATOM	8576	Ö	SER	349	109. 274	37. 739	23. 154	1.00 21.00	В	Ö	
ATOM	8577	N	THR	350	110.351	36. 112	24. 264	1.00 21.76	В	N	
ATOM	8578	CA	THR	350	109.654	35. 033	23. 571	1.00 23.08	В	Č	
ATOM	8579	CB	THR	350	110.603	33. 882	23. 214	1.00 22.77	B	č	
ATOM	8580	0G1		350	111.310	33. 483	24. 391	1.00 25.37	B	ŏ	•
ATOM	8581		THR	350	111.583	34. 299	22. 152	1.00 22.93	B	č	
ATOM	8582	C	THR	350	108.561	34. 453	24. 475	1.00 22.93	B	Č	
ATOM	8583	Ö	THR	350	107.732	33.650	24.035	1.00 20.70	В	0	
ATOM	8584	N	THR	351	108.564	34.871	25.737	1.00 22.30	В	N	
ATOM	8585	CA	THR	351	107.601	34.366	26.703	1.00 22.35	В	C	
ATOM	8586	CB	THR	351	108.332	33. 796	27.932	1.00 23.36	В	C	
ATOM	8587	0G1	THR	351	108.989	34.859	28. 635	1.00 25.67	В	0	
ATOM	8588		THR	351	109. 378	32. 781	27.493	1.00 22.26	В	C	
ATOM	8589	C	THR	351	106.575	35. 392	27. 171	1.00 21.07	В	C	
ATOM	8590	0	THR	351	105. 562	35.031	27. 760	1.00 20.87	В	0	
ATOM	8591	N	GLY	352	106.839	36.668	26. 918	1.00 19.83	В	N	
ATOM	8592	CA	GLY	352	105.894	37. 692	27. 325	1.00 19.36	В	C	
ATOM	8593	C	GLY	352	106.182	39. 027	26.672	1.00 18.63	В	C	
ATOM	8594	0	GLY	352	106.633	39.076	25.531	1.00 20.78	В	0	
ATOM	8595 8596	N	TRP TRP	353 353	105.913	40.109	27. 397	1.00 17.51	В	N	
ATOM ATOM	8597	CA CB	TRP	353	106. 156 105. 195	41.464 42.451	26. 907 27. 587	1.00 15.30 1.00 13.08	В	C	
ATOM	8598	CG	TRP	353 353	105. 165	42. 451	29. 084	1.00 13.08	B B	C	
ATOM	8599	CD2		353	104. 479	41.387	29. 877	1.00 7.79	В	C	
ATOM	8600	CE2		353	104. 739	41.684	31. 233	1.00 8.17	В	Č	
ATOM	8601	CE3		353	103.671	40. 288	29.574	1.00 10.72	B	č	
ATOM	8602	CD1		353	105. 798	43. 195	29.966	1.00 11.19	B	Č	
ATOM	8603		TRP	353	105. 546	42. 791	31. 265	1.00 10.10	B	Ň	
ATOM	8604	CZ2		353	104.217	40.921	32. 281	1.00 10.66	B	Ĉ	
ATOM	8605	CZ3	TRP	353	103.149	39. 524	30.625	1.00 10.40	В	Ċ	
ATOM	8606	CH2	TRP	353	103.426	39.848	31.958	1.00 9.81	В	C	
ATOM	8607	C	TRP	353	107. 594	41.796	27. 264	1.00.15.80	В	C	
ATOM	8608	0	TRP	353	108. 247	40. 999	27. 931	1.00 16.59	В	0	
ATOM	8609	N	VAL	354	108. 092	42.946	26.819	1.00 13.84	В	N	
ATOM	8610	CA	VAL	354	109.464	43. 338	27. 140	1.00 13.65	В	C	
ATOM	8611	CB	VAL	354	110. 135	44.096	25.960	1.00 16.06	В	C	
ATOM	8612	CG1		354	111.506	44. 646	26.400	1.00 12.56	В	Č	
ATOM	8613	CG2		354	110. 284	43. 163	24. 751	1.00 12.49	В	C	
ATOM	8614	C	VAL	354	109.486	44. 248	28. 368	1.00 13.83	В	C	
ATOM	8615	0	VAL	354	108. 716	45. 197	28. 456	1.00 13.93	В	0	
ATOM ATOM	8616 8617	N CA	GLY GLY	355	110.373	43.957	29. 313	1.00 14.87	В	И	
ATOM	8618	C	GLY	355 355	110. 467 109. 333	44.769	30.519	1.00 16.09	В	C	
ATOM	8619	0	GLY	355	109. 333	44. 554 43. 877	31.513 31.206	1.00 16.34 1.00 18.25	B B	C	
ATOM	8620	N	ARG	356	108. 341	45. 126	32. 706	1.00 15.25	В	O N	
ATOM	8621	CA	ARG	356	103. 404	44. 953	33. 701	1.00 15.10	В	C	
ATOM	8622	CB	ARG	356	108. 856	45. 494	35. 066	1.00 10.32	В	Č	
ATOM	8623	CG	ARG	356	110.001	44. 668	35.667	1.00 13.44	B	C	
					-					-	

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(Continued) FIG. 4-177 37.151 C **ATOM** 8624 CD ARG 356 110.169 44.878 1.00 14.42 111.546 45.211 37.511 1.00 18.65 N 8625 NE ATOM ARG 356 В 37.935 CZ 44.341 C ARG 112.457 1.00 20.17 ATOM 8626 356 В 38.065 NH1 ARG 112.156 43.055 1.00 22.71 N **ATOM** 8627 356 В 38. 242 NH2 ARG 113.674 44.765 1.00 18.93 N **ATOM** 8628 356 В 33. 209 33. 066 107. 111 45.607 1.00 16.01 C B ATOM 8629 C ARG 356 356 106.100 44.924 1.00 16.29 0 ATOM 8630 0 ARG 32.945 357 107.140 46.911 1.00 15.89 N ATOM 8631 N PHE B ATOM ATOM 105.967 32.402 8632 PHE 357 47.603 1.00 16.40 В C CA 105. 418 104. 753 33. 366 34. 573 48.660 1.00 11.21 C 8633 PHE 357 В CB48.083 1.00 8.48 ATOM 8634 CG PHE 357 В **ATOM** 8635 CD1 PHE 357 105.467 47.878 35.748 1.00 5.58 В C 103.407 **ATOM** 8636 CD2 PHE 357 47.711 34. 531 1.00 8.57 В C 104.846 36.867 ATOM 8637 CE1 PHE 357 47.309 1.00 5.98 В 102.777 35.648 C ATOM 8638 CE2 PHE 357 47.136 1.00 4.59 B 103.498 46.937 36.812 3.60 C ATOM 8639 CZPHE 357 1.00 В 106. 344 105. 476 ATOM C 48.259 31.076 1.00 18.69 C 8640 PHE 357 B ATOM 48.638 30.287 1.00 21.57 0 8641 0 PHE 357 В 48.377 30.840 **ATOM** 8642 N ARG 358 107.648 1.00 19.12 В N 48.953 29.612 **ATOM** 8643 CA ARG 358 108.188 1.00 19.47 В C 107.826 50.439 29.499 1.00 19.02 C ATOM 8644 CB ARG 358 В 51.346 C ATOM 8645 CG ARG 358 108.451 30.559 1.00 19.99 В 108.074 **ATOM** 8646 CD ARG 358 52.820 30.338 1.00 22.48 C В 108.633 53.708 31.362 **ATOM** 8647 NE ARG 358 1.00 24.20 В N 109. 204 109. 304 ATOM CZ358 54.890 31.117 1.00 24.69 8648 ARG В C ATOM 8649 ARG 358 55.358 29.875 1.00 21.14 NH1 В N ATOM 8650 ARG 109.696 55.603 32.121 1.00 24.33 NH2 358 В N 109. 707 110. 302 ATOM 48.784 29.646 1.00 20.57 В 8651 C ARG 358 C В ATOM 8652 ARG 358 48.704 30.722 1.00 22.16 0 0 ATOM 8653 PR₀ 359 110.355 48.723 28.473 1.00 20.23 В N N 109.783 ATOM 8654 CD PR₀ 359 48.894 27.124 1.00 20.61 В C 111.816 ATOM ATOM PRO PRO C 8655 CA 359 48.564 28.411 1.00 20.48 В 8656 CB 359 48.916 26.959 1.00 19.85 В C ATOM CG PR₀ 110.919 48.431 26.229 1.00 21.21 C 8657 359 В 112. 527 112. 221 ATOM C 49.494 29.402 1.00 20.23 C 8658 **PRO** 359 В 8659 0 **PRO** 50.683 29.465 В ATOM 359 1.00 22.01 0 **ATOM** 113.474 8660 N SER 360 48.953 30.163 1.00 19.33 В N 114. 212 115. 122 49.725 **ATOM** 8661 CA SER 360 31.160 1.00 18.75 В C ATOM 48.806 31.968 В 8662 CB SER 360 1.00 20.74 C **ATOM** 8663 116.163 1.00 26.03 В 0G SER 360 48.286 31.149 0 **ATOM** 115.060 30.560 1.00 18.77 8664 C SER 360 50.841 В C 115. 410 115. 394 29.382 1.00 17.99 ATOM 8665 0 50.806 В SER 360 0 **ATOM** 8666 **GLU** 31.393 1.00 18.96 B N 361 51.824 N **ATOM** 8667 GLU 116.199 52.970 30.978 CA 361 1.00 18.11 B C **ATOM** GLU 8668 CB 115.982 54.159 31.919 1.00 16.34 C 361 В GLU C ATOM CG 1.00 21.67 8669 361 116.654 54.007 33.269 В ATOM 8670 CD GLU 361 115.743 53.431 34.342 1.00 27.42 В C

54.009 **SUBSTITUTE SHEET (RULE 26)**

52.408

34.091

35. 453

1.00 28.62

1.00 31.11

В

В

0

115.067

115.710

ATOM

ATOM

8671

8672

OE1 GLU

OE2 GLU

361

361

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					(Continued)
				FIG. 4-178	
ATOM	8673	C GLI	361	117.674 52.595 31.007 1.00 16.97 B	С
ATOM	8674	0 GLU		118.118 51.870 31.888 1.00 16.23 B	0
ATOM	8675	N PRO		118.449 53.079 30.030 1.00 16.09 B	N
ATOM	8676	CD PRO		118. 027 53. 805 28. 817 1. 00 13. 66 B	C
ATOM	8677	CA PRO		119. 879 52. 772 29. 985 1. 00 15. 32 B	C
ATOM	8678	CB PRO		120. 207 52. 916 28. 505 1. 00 13. 19 B 119. 362 54. 086 28. 121 1. 00 12. 78 B	C C
ATOM ATOM	8679 8680	C PRO		119.362 54.086 28.121 1.00 12.78 B 120.601 53.806 30.832 1.00 16.34 B	C
ATOM	8681	0 PR		120.096 54.911 31.021 1.00 17.05 B	0
ATOM	8682	N HIS		121.768 53.448 31.353 1.00 17.21 B	Ň
ATOM	8683	CA HIS		122.550 54.374 32.164 1.00 18.58 B	Ċ
ATOM	8684	CB HIS		122.626 53.875 33.603 1.00 18.05 B	Č
ATOM	8685	CG HIS		121. 324 53. 965 34. 333 1. 00 19. 33 B	C
ATOM	8686	CD2 HIS		120. 156 53. 301 34. 158 1. 00 19. 36 B	C
ATOM	8687	ND1 HIS		121.111 54.851 35.368 1.00 18.40 B	N
ATOM	8688	CE1 HIS		119. 869 54. 731 35. 799 1. 00 19. 50 B	C
ATOM	8689	NE2 HIS		119. 267 53. 798 35. 081 1. 00 22. 85 B	N
ATOM	8690	C HIS		123. 942 54. 499 31. 551 1. 00 19. 40 B	C
ATOM ATOM	8691 8692	O HIS		124. 833 53. 691 31. 806 1. 00 19. 73 B 124. 110 55. 520 30. 723 1. 00 19. 14 B	O N
ATOM	8693	CA PHE		125. 371 55. 744 30. 043 1. 00 19. 25 B	C
ATOM	8694	CB PHE		125.188 56.802 28.944 1.00 17.71 B	Č
ATOM	8695	CG PHE		124.368 56.319 27.777 1.00 15.99 B	č
ATOM	8696	CD1 PHE		122. 975 56. 339 27. 826 1. 00 12. 83 B	Č
ATOM	8697	CD2 PHE	364	124. 989 55. 770 26. 656 1. 00 12. 86 B	С
ATOM	8698	CE1 PHE		122. 216 55. 816 26. 781 1. 00 8. 09 B	C
ATOM	8699	CE2 PHE		124. 225 55. 242 25. 607 1. 00 10. 87 B	C .
ATOM	8700	CZ PHE		122.837 55.268 25.679 1.00 7.69 B	C
ATOM	8701	C PHE		126. 531 56. 127 30. 942 1. 00 18. 72 B	C
ATOM ATOM	8702 8703	O PHIE		126. 341 56. 638 32. 050 1. 00 17. 88 B 127. 735 55. 854 30. 448 1. 00 18. 23 B	0
ATOM	8704	CA THE		127. 735 55. 854 30. 448 1. 00 18. 23 B 128. 967 56. 178 31. 159 1. 00 19. 73 B	N C
ATOM	8705	CB THE		130. 132 55. 288 30. 697 1. 00 17. 73 B	č
ATOM	8706	OG1 THE		130. 257 55. 384 29. 275 1. 00 22. 16 B	ŏ
ATOM	8707	CG2 THE		129.890 53.848 31.069 1.00 13.36 B	č
ATOM	8708	C THE		129. 312 57. 633 30. 847 1. 00 20. 48 B	Č
ATOM	8709	0 THE		128. 662 58. 260 30. 015 1. 00 20. 68 B	0
ATOM	8710	N LEU		130. 329 58. 163 31. 515 1. 00 22. 60 B	N
ATOM	8711	CA LEU		130. 740 59. 544 31. 304 1. 00 25. 75 B	C
ATOM	8712	CB LEU		132. 053 59. 831 32. 039 1. 00 29. 32 B	C
ATOM	8713	CG LEU		132. 172 59. 429 33: 516 1. 00 34. 01 B	C
ATOM ATOM	8714	CD1 LEU		132.442 57.920 33.631 1.00 33.57 B	C
ATOM ATOM	8715 8716	CD2 LEU		133.316 60.210 34.162 1.00 34.78 B 130.909 59.900 29.824 1.00 26.20 B	C C
ATOM	8717	0 LEU		130. 317 60. 871 29. 349 1. 00 26. 53 B	0
ATOM	8718	N ASP		131. 709 59. 115 29. 102 1. 00 24. 26 B	N N
ATOM	8719	CA ASP		131.964 59.369 27.682 1.00 23.63 B	Č
ATOM	8720	CB ASP		133. 232 58. 636 27. 214 1. 00 23. 47 B	Č
ATOM	8721	CG ASF		133. 230 57. 158 27. 582 1. 00 25. 27 B	C
				61 1 5 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	

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				FIC 4-170	(Continued)
40014	0700	OD1 40D	0.07	FIG. 4-179	0
ATOM	8722	OD1 ASP	367	132. 158 56. 515 27. 507 1. 00 24. 35 B	0
ATOM ATOM	8723 8724	OD2 ASP C ASP	367 367	134.311 56.634 27.935 1.00 25.99 B 130.810 58.990 26.767 1.00 22.76 B	0 C
ATOM	8725	0 ASP	367	130. 848 59. 261 25. 568 1. 00 24. 31 B	0
ATOM	8726	N GLY	368	129. 795 58. 348 27. 330 1. 00 20. 91 B	Ň
ATOM	8727	CA GLY	368	128. 646 57. 950 26. 547 1. 00 18. 80 B	Ċ
ATOM	8728	C GLY	368	128. 912 56. 843 25. 550 1. 00 19. 81 B	č
ATOM	8729	0 GLY	368	128. 059 56. 563 24. 700 1. 00 19. 55 B	Ŏ
ATOM	8730	N ASN	369	130. 073 56. 198 25. 643 1. 00 19. 20 B	N
ATOM	8731	CA ASN	369	130. 398 55. 117 24. 706 1. 00 19. 60 B	C
ATOM	8732	CB ASN	369	131. 907 54. 986 24. 526 1. 00 19. 65 B	C
ATOM-	8733	CG ASN	369	132. 519 56. 217 23. 921 1. 00 21. 94 B	C
ATOM	8734	OD1 ASN	369	132.005 56.757 22.945 1.00 25.32 B	0
ATOM	8735	ND2 ASN	369	133. 628 56. 671 24. 489 1. 00 23. 16 B	Ŋ
ATOM	8736	C ASN	369	129. 828 53. 760 25. 090 1. 00 18. 53 B	C
ATOM	8737	O ASN	369	129. 770 52. 861 24. 258 1. 00 18. 17 B	0
ATOM	8738	N SER	370	129. 420 53. 608 26. 346 1. 00 18. 61 B	N
ATOM ATOM	8739 8740	CA SER CB SER	370 370	128. 847 52. 347 26. 812 1. 00 19. 50 B 129. 934 51. 447 27. 430 1. 00 20. 45 B	C C
ATOM	8741	OG SER	370	130.577 52.057 28.538 1.00 22.81 B	0
ATOM	8742	C SER	370	127. 746 52. 621 27. 829 1. 00 18. 95 B	Č
ATOM	8743	0 SER	370	127. 562 53. 759 28. 261 1. 00 19. 22 B	Ö
ATOM	8744	N PHE	371	127. 009 51. 583 28. 209 1. 00 18. 63 B	Ň
ATOM	8745	CA PHE	371	125. 931 51. 763 29. 168 1. 00 18. 66 B	Ċ
ATOM	8746	CB PHE	371	124. 762 52. 516 28. 512 1. 00 19. 79 B	Č
ATOM	8747	CG PHE	371	124. 088 51. 756 27. 398 1. 00 16. 47 B	Ċ
ATOM	8748	CD1 PHE	371	124. 532 51. 874 26. 093 1. 00 15. 63 B	C.
ATOM	8749	CD2 PHE	371	122. 991 50. 940 27. 660 1. 00 17. 78 B	C
ATOM	8750	CE1 PHE	371	123. 893 51. 198 25. 059 1. 00 18. 99 B	C
ATOM	8751	CE2 PHE	371	122. 340 50. 255 26. 631 1. 00 18. 61 B	C
ATOM	8752	CZ PHE	371	122. 792 50. 386 25. 327 1. 00 18. 10 B	C
ATOM ATOM	8753 8754	C PHE O PHE	371	125. 402 50. 473 29. 784 1. 00 18. 78 B	C
ATOM	8755	O PHE N TYR	371 372	125. 506 49. 392 29. 197 1. 00 17. 45 B 124. 814 50. 614 30. 970 1. 00 19. 00 B	0
ATOM	8756	CA TYR	372	124. 814 50. 614 30. 970 1. 00 19. 00 B 124. 240 49. 491 31. 703 1. 00 18. 59 B	N C
ATOM	8757	CB TYR	372	124. 697 49. 527 33. 159 1. 00 17. 86 B	C C
ATOM	8758	CG TYR	372	126. 199 49. 500 33. 290 1. 00 17. 83 B	C
ATOM	8759	CD1 TYR	372	126. 951 50. 676 33. 201 1. 00 19. 52 B	Č
ATOM	8760	CE1 TYR	372	128. 339 50. 651 33. 257 1. 00 18. 29 B	č
ATOM	8761	CD2 TYR	372	126. 878 48. 296 33. 441 1. 00 17. 45 B	č
ATOM	8762	CE2 TYR	372	128. 266 48. 257 33. 498 1. 00 18. 99 B	Č
ATOM	8763	CZ TYR	372	128.991 49.434 33.405 1.00 18.83 B	Ċ
ATOM	8764	OH TYR	372	130. 364 49. 387 33. 454 1. 00 19. 89 B	0
ATOM	8765	C TYR	372	122. 727 49. 558 31. 620 1. 00 18. 38 B	C
ATOM	8766	O TYR	372	122.143 50.632 31.717 1.00 20.19 B	0
ATOM	8767	N LYS	373	122.096 48.406 31.436 1.00 19.10 B	N
ATOM ATOM	8768 8769	CA LYS	373	120. 647 48. 340 31. 299 1. 00 18. 51 B	C
ATOM	8770	CB LYS	373	120. 285 48. 376 29. 809 1. 00 17. 90 B	C
UTOM	0110	CG LYS	373	118. 809 48. 581 29. 485 1. 00 21. 01 B	С

					_			4.0.0				(Con	tinued)
					F	I G	. 4 -	180					
ATOM	8771	CD	LYS	373	118. 5		48. 627	27.969		21.40	В	C	
ATOM	8772	CE	LYS	373	117. 2		49. 238	27. 563		21.67	В	C	
ATOM	8773	ΝZ	LYS	373	116.0		48. 389	27. 855		21.98	В	N	
ATOM	8774	C	LYS	373	120.1		47.049	31. 928		18.77	В	C	
ATOM	8775	0	LYS	373	120.6	95	45. 980	31.712		18.48 17.06	B B	O N	
ATOM	8776	N	ILE	374	119. 0 118. 4	00 74	47. 150 45. 972	32. 709 33. 332		15.88	В	C	
ATOM	8777	CA	ILE	374 374	117. 5		46. 339	34. 526		14.58	В	C	
ATOM	8778 8779	CB CG2	ILE	374	116.9		45.076	35. 130		12.18	В	C	
ATOM ATOM	8780	CG2		374	118.3		47. 101	35. 591		15.07	В	Č	
ATOM	8781	CD1		374	117. 5		47. 505	36.809		13.03	В	č	
ATOM	8782	CDI	ILE	374	117.6		45. 244	32. 303		16.94	B	č	
ATOM	8783	ŏ	ILE	374	116.6		45. 803	31. 795		17.41	B	Ŏ	
ATOM	8784	N	ILE	375	117. 9		44.008	31. 978		18.50	В	N	
ATOM	8785	ĊA	ILE	375	117. 1		43. 226	31.033		19.71	В	C	
ATOM	8786	CB	ILE	375	117.8		43.117	29.625		19.62	В	C	
ATOM	8787	CG2		375	118.1		44. 496	29.070	1.00	19.13	В	C	
ATOM	8788	CG1		375	119. 1		42. 298	29.706	1.00	21.23	В	C	
ATOM	8789	CD1	ILE	375	119.8		42.129	28. 373		23.06	В	C	
ATOM	8790	C	ILE	375	116.9		41.815	31.579		20.44	В	C	
ATOM	8791	0	ILE	375	117.7		41.356	32.443		20.03	В	0	
ATOM	8792	N	SER	376	115. 9	68	41.128	31.078		21.14	В	N	
ATOM	8793	CA	SER	376	115. 7		39. 771	31.516		21.95	В	Č	
ATOM	8794	CB	SER	376	114. 3	47	39. 318	31.003		21.55	В	C	
ATOM	8795	0G	SER	376	114.0		38. 054	31.539		25. 40	В	0	
ATOM	8796	C	SER	376	116.8		38. 899	30. 936		23.06	В	C	
ATOM	8797	0	SER	376	117. 2		39. 127	29. 807		24. 16	В	0	
ATOM	8798	N	ASN	377	117. 2		37. 914	31.698		24. 67	В	N	
ATOM	8799	CA	ASN	377	118. 3		37. 053	31.218		25.07	В	C	
ATOM	8800	CB CG	ASN ASN	377 377	119. 4 119. 0		36. 891 35. 971	32. 302 33. 444		23. 49 23. 86	B B	C.	
ATOM ATOM	8801 8802	0D1		377	117. 9		35. 340	33. 397		23. 70	В	0	
ATOM	8803	ND2		377	119.8		35. 884	34. 474		20.11	В	N	
ATOM	8804	C	ASN	377	117.8		35. 681	30. 736		26.79	В	Č	
ATOM	8805	ŏ	ASN	377	116.7		35. 382	30. 699		28. 58	B	ŏ	
ATOM	8806	N	GLU	378	118.8		34. 856	30. 353		29. 97	B	N	
ATOM	8807	CA	GLU	378	118. 6		33. 504	29. 871		33. 15	B	Ċ	
ATOM	8808	CB	GLU	378	119. 9		32. 716	29. 870		37. 08	B	č	
ATOM	8809	ĊĠ	GLU	378	120. 6		32.870	31. 181		43. 78	B	Č	
ATOM	8810	CD	GLU	378	121.6		31.740	31.427		46.56	В	Č	
ATOM	8811		GLU	378	121. 2		30.613	31.725		47.52	В	0	
ATOM	8812	0E2		378	122. 9		31.981	31.321		47.91	В	0	
ATOM	8813	C	GLU	378	117. 5		32.760	30. 722		33.63	В	C	
ATOM	8814	0	GLU	378	116.6		32.113	30. 192		35. 16	В	0	
ATOM	8815	N	GLU	379	117.7		32.842	32.041		32. 70	В	N	
ATOM	8816	CA	GLU	379	116.8		32. 160	32. 953		30.44	В	C	
ATOM	8817	CB	GLU	379	117. 5		31.806	34. 256		34. 46	В	C	
ATOM	8818	CG	GLU	379	117. 8		30. 323	34. 412		39.45	В	C	
ATOM	8819	CD	GLU	379	116.5	77	29. 475	34. 492	1.00	43. 32	В	C	

				FIG. 4-181	(Continued	ł)
ATOM	8820	OE1 GLU	379	115.800 29.642 35.463 1.00 42.91 B	0	
ATOM	8821	OE2 GLU	379	116. 357 28. 643 33. 580 1. 00 45. 81 B	0	
ATOM	8822	C GLU	379	115.588 32.972 33.265 1.00 28.15 B	С	
ATOM	8823	0 GLU	379	114.743 32.539 34.049 1.00 28.12 B	0	
ATOM	8824	N GLY	380	115. 473 34. 148 32. 658 1. 00 24. 72 B	N	
ATOM	8825	CA GLY	380	114. 304 34. 980 32. 886 1. 00 22. 38 B	С	
ATOM	8826	C GLY	380	114. 335 35. 891 34. 101 1. 00 21. 23 B	С	
ATOM	8827	0 GLY	380	113. 302 36. 404 34. 514 1. 00 21. 76 B	0	
ATOM	8828	N TYR	381	115. 507 36. 084 34. 689 1. 00 20. 24 B	N	
ATOM	8829	CA TYR	381	115.642 36.963 35.842 1.00 19.52 B	Č	
ATOM	8830	CB TYR	381	116.539 36.307 36.884 1.00 20.98 B	C	
ATOM	8831	CG TYR	381	115. 846 35. 194 37. 630 1. 00 23. 80 B	C	
ATOM	8832	CD1 TYR	381	115. 104 35. 465 38. 781 1. 00 23. 87 B	C	
ATOM ATOM	8833 8834	CE1 TYR CD2 TYR	381	114. 435 34. 458 39. 455 1. 00 22. 94 B	C C C	
ATOM	8835	CE2 TYR	381 381	115. 900 33. 876 37. 171 1. 00 22. 81 B 115. 232 32. 859 37. 843 1. 00 22. 55 B	C	
ATOM	8836	CZ TYR	381	115. 232 32. 859 37. 843 1. 00 22. 55 B 114. 501 33. 161 38. 986 1. 00 24. 14 B	C	
ATOM	8837	OH TYR	381	113. 830 32. 170 39. 667 1. 00 25. 04 B	0	
ATOM	8838	C TYR	381	116. 237 38. 292 35. 374 1. 00 19. 14 B	C	
ATOM	8839	0 TYR	381	117. 178 38. 312 34. 568 1. 00 18. 95 B	0	
ATOM	8840	N ARG	382	115. 689 39. 399 35. 871 1. 00 15. 40 B	N .	
ATOM	8841	CA ARG	382	116. 160 40. 715 35. 458 1. 00 14. 04 B	Č	
ATOM	8842	CB ARG	382	115.035 41.738 35.622 1.00 13.48 B	č	
ATOM	8843	CG ARG	382	113.948 41.478 34.606 1.00 15.55 B	Č	
ATOM	8844	CD ARG	382	112.581 42.001 34.993 1.00 17.88 B	C	
ATOM	8845	NE ARG	382	111.576 41.337 34.170 1.00 19.19 B	N	
ATOM	8846	CZ ARG	382	111. 438 41. 515 32. 859 1. 00 21. 25 B	С	
ATOM	8847	NH1 ARG	382	112. 230 42. 357 32. 203 1. 00 18. 86 B	N	
ATOM	8848	NH2 ARG	382	110. 534 40. 810 32. 190 1. 00 23. 20 B	N ·	
ATOM	8849	C ARG	382	117. 438 41. 172 36. 140 1. 00 12. 33 B	C	
ATOM	8850	0 ARG	382	117. 497 41. 376 37. 349 1. 00 9. 83 B	0	
ATOM ATOM	8851 8852	N HIS CA HIS	383	118. 474 41. 303 35. 323 1. 00 11. 97 B	N	
ATOM	8853	CB HIS	383 383	119. 778 41. 711 35. 789 1. 00 12. 81 B 120. 714 40. 516 35. 777 1. 00 12. 29 B	C	
ATOM	8854	CG HIS	383		C	
ATOM	8855	CD2 HIS	383	120. 377 39. 496 36. 813 1. 00 13. 83 B 119. 726 38. 313 36. 721 1. 00 12. 69 B	C C	
ATOM		ND1 HIS	383	120. 670 39. 675 38. 148 1. 00 13. 84 B	N	
ATOM	8857	CE1 HIS	383	120. 212 38. 643 38. 834 1. 00 16. 23 B	C	
ATOM	8858	NE2 HIS	383	119.635 37.803 37.993 1.00 14.04 B	N .	
ATOM	8859	C HIS	383	120. 351 42. 830 34. 949 1. 00 14. 10 B	C	
ATOM	8860	0 HIS	383	119. 788 43. 207 33. 913 1. 00 15. 53 B	Ö	
ATOM	8861	N ILE	384	121. 476 43. 354 35. 412 1. 00 13. 75 B	Ň	
ATOM	8862	CA ILE	384	122. 166 44. 444 34. 749 1. 00 15. 78 B	Ċ	
ATOM	8863	CB ILE	384	122. 996 45. 223 35. 782 1. 00 14. 50 B	C C C	
ATOM	8864	CG2 ILE	384	123. 765 46. 338 35. 103 1. 00 14. 15 B	С	
ATOM	8865	CG1 ILE	384	122. 071 45. 767 36. 871 1. 00 12. 97 B	С	
ATOM	8866	CD1 ILE	384	122. 791 46. 194 38. 129 1. 00 14. 46 B	C	
ATOM	8867	C ILE	384	123. 082 43. 925 33. 645 1. 00 18. 38 B	C	
ATOM	8868	0 ILE	384	123. 884 43. 014 33. 874 1. 00 20. 02 B	0	

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										(Continued)
					FIC	3. 4	- 182),		Continued
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	8869 8870 8871 8872 8873 8874 8875 8876	CA C C CB CB CA CA	CYS CYS CYS CYS TYR TYR	385 385 385 385 385 386 386 386	122. 956 123. 812 124. 628 124. 115 122. 980 123. 868 125. 908 126. 795 128. 222	44. 485 44. 063 45. 266 46. 376 43. 476 42. 151 45. 046 46. 111 45. 849	32. 446 31. 340 30. 868 30. 775 30. 178 29. 269 30. 595 30. 138	1.00 19.06 1.00 20.78 1.00 19.29 1.00 19.30 1.00 22.83 1.00 35.68 1.00 18.55	B B B B B B	N C C O C S N C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM	8878 8879 8880 8881 8882 8883 8884	CD CE CD: CE: CZ OH	1 TYR 1 TYR 2 TYR 2 TYR TYR TYR	386 386 386 386 386 386	129. 224 130. 557 131. 504 128. 857 129. 798 131. 127 132. 082	46. 938 46. 620 47. 602 48. 276 49. 274 48. 925 49. 894	30. 049 29. 797 30. 279 30. 032 29. 791 29. 561	1.00 17.08 1.00 18.50 1.00 20.09 1.00 17.91 1.00 21.21 1.00 21.94 1.00 21.36	B B B B B	C C C C C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM	8885 8886 8887 8888 8889 8890 8891		TYR TYR PHE PHE PHE PHE PHE	386 386 387 387 387 387 387	125.161	46. 116 45. 069 47. 291 47. 418 47. 939 47. 000 46. 373	28. 625 28. 004 28. 035 26. 587 26. 133 26. 347 25. 258	1. 00 17. 85 1. 00 18. 61 1. 00 18. 83 1. 00 17. 08 1. 00 14. 86 1. 00 14. 70	B B B B B	C O N C C C C
ATOM ATOM ATOM ATOM ATOM	8892 8893 8894 8895 8896 8897	CE1 CE2 CZ C C	PHE PHE PHE PHE PHE	387 387 387 387 387 387	123. 444 122. 246 122. 283 121. 680 127. 552 127. 859	46. 848 45. 624 46. 100 45. 491 48. 408 49. 413	27. 605 25. 419 27. 777 26. 684 26. 057 26. 706	1. 00 12. 48 1. 00 13. 25 1. 00 11. 47 1. 00 12. 33 1. 00 21. 93 1. 00 20. 79	B B B B	C C C C C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM	8898 8899 8900 8901 8902 8903	NE2	GLN GLN GLN GLN GLN GLN GLN	388 388 388 388 388 388	128. 994 130. 122 130. 905 131. 787 132. 672 131. 553	48. 113 48. 970 48. 140 47. 326 48. 185 48. 871 48. 160	24. 859 24. 137 23. 534 24. 542 25. 401 24. 898 26. 705	1. 00 24. 26 1. 00 26. 10 1. 00 26. 78 1. 00 28. 07 1. 00 27. 71 1. 00 30. 29 1. 00 30. 63	B B B B B	N C C C C O N
ATOM ATOM ATOM ATOM ATOM ATOM ATOM	8905 8906 8907 8908 8909 8910		GLN GLN ILE ILE ILE ILE	388 388 389 389 389	128. 074 127. 300 128. 130 127. 224 127. 233 126. 839	49. 474 48. 690 50. 755 51. 256 52. 796 53. 374	23. 024 22. 478 22. 681 21. 650 21. 576 22. 933	1. 00 28. 20 1. 00 28. 61 1. 00 30. 33 1. 00 32. 95 1. 00 29. 60 1. 00 27. 56	B B B B	C O N C C
ATOM ATOM ATOM ATOM ATOM ATOM	8911 8912 8913 8914 8915 8916 8917		ILE ILE ILE ILE ASP ASP ASP	389 389 389 389 390 390	128. 699	53. 296 54. 810 50. 692 50. 705 50. 184 49. 621 50. 005	21. 129 21. 005 20. 261 19. 404 20. 039 18. 741 18. 365	1.00 27.72 1.00 26.00 1.00 37.72 1.00 40.02 1.00 41.52 1.00 43.97 1.00 45.79	B B B B B	C C C O N C

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ATOM 8967 CD2 PHE 396 123.265 38.378 30.837 1.00 19.67 B C ATOM 8968 CE1 PHE 396 121.267 40.157 31.593 1.00 21.82 B C ATOM 8969 CE2 PHE 396 122.062 38.411 30.130 1.00 20.02 B C ATOM 8970 CZ PHE 396 121.057 39.303 30.507 1.00 22.36 B C ATOM 8971 C PHE 396 126.712 40.596 33.488 1.00 19.09 B C ATOM 8972 O PHE 396 127.703 39.866 33.516 1.00 21.70 B O ATOM 8973 N ILE 397 126.511 41.559 34.380 1.00 17.18 B N ATOM 8974 CA ILE 397 127.454 41.774 35.460 1.00 14.91 B C ATOM 8975 CB ILE 397 127.819 43.240 35.566 1.00 14.47 B C ATOM 8976 CG2 ILE 397 128.181 43.762 34.192 1.00 14.09 B C	ed)
ATOM 8968 CE1 PHE 396 121.267 40.157 31.593 1.00 21.82 B C ATOM 8969 CE2 PHE 396 122.062 38.411 30.130 1.00 20.02 B C ATOM 8970 CZ PHE 396 121.057 39.303 30.507 1.00 22.36 B C ATOM 8971 C PHE 396 126.712 40.596 33.488 1.00 19.09 B C ATOM 8972 O PHE 396 127.703 39.866 33.516 1.00 21.70 B O ATOM 8973 N ILE 397 126.511 41.559 34.380 1.00 17.18 B N ATOM 8974 CA ILE 397 127.454 41.774 35.460 1.00 14.91 B C ATOM 8975 CB ILE 397 127.819 43.240 35.566 1.00 14.47 B C	
ATOM 8968 CE1 PHE 396 121.267 40.157 31.593 1.00 21.82 B C ATOM 8969 CE2 PHE 396 122.062 38.411 30.130 1.00 20.02 B C ATOM 8970 CZ PHE 396 121.057 39.303 30.507 1.00 22.36 B C ATOM 8971 C PHE 396 126.712 40.596 33.488 1.00 19.09 B C ATOM 8972 O PHE 396 127.703 39.866 33.516 1.00 21.70 B O ATOM 8973 N ILE 397 126.511 41.559 34.380 1.00 17.18 B N ATOM 8974 CA ILE 397 127.454 41.774 35.460 1.00 14.91 B C ATOM 8975 CB ILE 397 127.819 43.240 35.566 1.00 14.47 B C	
ATOM 8969 CE2 PHE 396 122.062 38.411 30.130 1.00 20.02 B C ATOM 8970 CZ PHE 396 121.057 39.303 30.507 1.00 22.36 B C ATOM 8971 C PHE 396 126.712 40.596 33.488 1.00 19.09 B C ATOM 8972 O PHE 396 127.703 39.866 33.516 1.00 21.70 B O ATOM 8973 N ILE 397 126.511 41.559 34.380 1.00 17.18 B N ATOM 8974 CA ILE 397 127.454 41.774 35.460 1.00 14.91 B C ATOM 8975 CB ILE 397 127.819 43.240 35.566 1.00 14.47 B C	
ATOM 8971 C PHE 396 126.712 40.596 33.488 1.00 19.09 B C ATOM 8972 O PHE 396 127.703 39.866 33.516 1.00 21.70 B O ATOM 8973 N ILE 397 126.511 41.559 34.380 1.00 17.18 B N ATOM 8974 CA ILE 397 127.454 41.774 35.460 1.00 14.91 B C ATOM 8975 CB ILE 397 127.819 43.240 35.566 1.00 14.47 B C	
ATOM 8972 O PHE 396 127.703 39.866 33.516 1.00 21.70 B O ATOM 8973 N ILE 397 126.511 41.559 34.380 1.00 17.18 B N ATOM 8974 CA ILE 397 127.454 41.774 35.460 1.00 14.91 B C ATOM 8975 CB ILE 397 127.819 43.240 35.566 1.00 14.47 B C	
ATOM 8973 N ILE 397 126.511 41.559 34.380 1.00 17.18 B N ATOM 8974 CA ILE 397 127.454 41.774 35.460 1.00 14.91 B C ATOM 8975 CB ILE 397 127.819 43.240 35.566 1.00 14.47 B C	
ATOM 8974 CA ILE 397 127.454 41.774 35.460 1.00 14.91 B C ATOM 8975 CB ILE 397 127.819 43.240 35.566 1.00 14.47 B C	
ATOM 8975 CB ILE 397 127.819 43.240 35.566 1.00 14.47 B C	
ATOM 8978 CD1 ILE 397 126.993 45.472 36.449 1.00 11.32 B C ATOM 8979 C ILE 397 126.885 41.287 36.791 1.00 16.82 B C	
ATOM 8980 0 ILE 397 127.543 41.376 37.833 1.00 18.48 B 0	
ATOM 8981 N THR 398 125.651 40.790 36.753 1.00 15.47 B N	
ATOM 8982 CA THR 398 125.000 40.241 37.937 1.00 14.86 B C	
ATOM 8983 CB THR 398 124.049 41.255 38.652 1.00 14.72 B C	
ATOM 8984 OG1 THR 398 122.968 41.627 37.784 1.00 13.55 B O	
ATOM 8985 CG2 THR 398 124.812 42.476 39.083 1.00 13.88 B C	
ATOM 8986 C THR 398 124.185 39.040 37.490 1.00 15.72 B C	
ATOM 8987 0 THR 398 123.805 38.942 36.323 1.00 15.48 B 0	
ATOM 8988 N LYS 399 123.915 38.127 38.416 1.00 17.12 B N	
ATOM 8989 CA LYS 399 123.147 36.935 38.094 1.00 18.19 B C	
ATOM 8990 CB LYS 399 124.026 35.960 37.314 1.00 20.96 B C	
ATOM 8991 CG LYS 399 125.322 35.630 38.023 1.00 24.93 B C	
ATOM 8992 CD LYS 399 125.970 34.380 37.458 1.00 29.93 B C	
ATOM 8993 CE LYS 399 127.055 33.860 38.402 1.00 32.81 B C ATOM 8994 NZ LYS 399 128.082 34.904 38.703 1.00 34.86 B N	
ATOM 8994 NZ LYS 399 128.082 34.904 38.703 1.00 34.86 B N ATOM 8995 C LYS 399 122.616 36.259 39.354 1.00 17.75 B C	
ATOM 8996 0 LYS 399 123.041 36.571 40.465 1.00 18.35 B 0	
ATOM 8997 N GLY 400 121.684 35.331 39.181 1.00 16.55 B N	
ATOM 8998 CA GLY 400 121.131 34.640 40.327 1.00 17.62 B C	
ATOM 8999 C GLY 400 119.616 34.629 40.320 1.00 19.66 B C	
ATOM 9000 0 GLY 400 118.979 35.360 39.551 1.00 22.36 B 0	
ATOM 9001 N THR 401 119.028 33.797 41.172 1.00 18.45 B N	
ATOM 9002 CA THR 401 117.582 33.708 41.227 1.00 17.93 B C	
ATOM 9003 CB THR 401 117.125 32.323 41.700 1.00 17.98 B C	
ATOM 9004 OG1 THR 401 117.653 32.056 43.004 1.00 20.05 B 0	
ATOM 9005 CG2 THR 401 117.607 31.267 40.730 1.00 13.15 B C	
ATOM 9006 C THR 401 117.013 34.785 42.125 1.00 16.85 B C	
ATOM 9007 0 THR 401 116. 478 34. 519 43. 192 1. 00 18. 14 B 0	
ATOM 9008 N TRP 402 117. 155 36. 013 41. 659 1. 00 16. 42 B N	
ATOM 9009 CA TRP 402 116.671 37.199 42.335 1.00 14.66 B C	
ATOM 9010 CB TRP 402 117.528 37.503 43.561 1.00 16.17 B C ATOM 9011 CG TRP 402 119.001 37.502 43.296 1.00 16.85 B C	
ATOM 9011 CG TRP 402 119.001 37.502 43.296 1.00 16.85 B C ATOM 9012 CD2 TRP 402 119.793 38.614 42.861 1.00 17.78 B C	
ATOM 9012 CD2 TRP 402 119.793 38.014 42.001 1.00 17.70 B C	
ATOM 9014 CE3 TRP 402 119.504 39.948 42.542 1.00 18.13 B C	
ATOM 9015 CD1 TRP 402 119.859 36.453 43.440 1.00 16.20 B C	

				·	4
			•	EIC 4-195	(Continued)
				FIG. 4-185	
ATOM	9016	NE1 TRP	402	121.143 36.842 43.130 1.00 18.41	B N
ATOM	9017	CZ2 TRP	402	122. 180 39. 003 42. 378 1. 00 16. 56	ВС
ATOM	9018	CZ3 TRP	402	120. 553 40. 784 42. 151 1. 00 18. 56	B C
ATOM	9019	CH2 TRP	402	121.874 40.303 42.075 1.00 17.33	B C
ATOM	9020	C TRP	402	116.827 38.280 41.273 1.00 14.94	ВС
ATOM	9021	0 TRP	402	117. 439 38. 022 40. 229 1. 00 14. 00	B . 0
ATOM	9022	N GLU	403	116. 309 39. 480 41. 534 1. 00 13. 41	B N
ATOM	9023	CA GLU	403	116.368 40.554 40.548 1.00 12.05	B C
ATOM	9024	CB GLU	403	114.990 40.703 39.899 1.00 10.24	B C
ATOM	9025	CG GLU	403	114. 408 39. 396 39. 398 1. 00 10. 20	B C
ATOM	9026	CD GLU	403	113. 288 39. 607 38. 391 1. 00 14. 00	ВС
ATOM	9027	OE1 GLU	403	112. 301 40. 306 38. 713 1. 00 15. 50	B 0
ATOM	9028	OE2 GLU	403	113. 397 39. 068 37. 271 1. 00 14. 63	B 0
ATOM	9029	C GLU	403	116. 852 41. 938 40. 999 1. 00 13. 29	B C
ATOM	9030	O GLU	403	116. 785 42. 301 42. 171 1. 00 14. 74	B 0
ATOM	9031	N VAL	404	117. 322 42. 716 40. 031 1. 00 12. 89	B N
ATOM	9032	CA VAL	404	117. 800 44. 067 40. 270 1. 00 12. 91	B C
ATOM	9033	CB VAL	404	118. 926 44. 420 39. 265 1. 00 11. 91	B C
ATOM	9034	CG1 VAL	404	119. 374 45. 859 39. 453 1. 00 13. 92	B C
ATOM	9035	CG2 VAL	404	120.096 43.484 39.459 1.00 8.31	B C B C
ATOM	9036	C VAL	404	116.607 44.994 40.039 1.00 14.23 116.129 45.105 38.918 1.00 16.13	B C B O
ATOM ATOM	9037 9038	O VAL N ILE	404 405	116.129 45.105 38.918 1.00 16.13 116.122 45.653 41.089 1.00 13.56	B N
ATOM	9039	CA ILE	405	114.968 46.540 40.951 1.00 12.56	B C
ATOM	9040	CB ILE	405	114. 453 47. 020 42. 339 1. 00 12. 98	B C
ATOM	9041	CG2 ILE	405	113. 151 47. 763 42. 183 1. 00 7. 46	B C
ATOM	9042	CG1 ILE	405	114. 256 45. 824 43. 282 1. 00 14. 03	B C
ATOM	9043	CD1 ILE	405		B C
ATOM	9044	C ILE	405	115. 293 47. 762 40. 088 1. 00 14. 39	B C
ATOM	9045	0 ILE	405	114.504 48.156 39.226 1.00 14.58	B 0
ATOM	9046	N GLY	406	116.455 48.367 40.315 1.00 14.30	B N
ATOM	9047	CA GLY	406	116.822 49.521 39.521 1.00 12.80	ВС
ATOM	9048	C GLY	406	118. 253 49. 967 39. 708 1. 00 13. 75	B C
ATOM	9049	O GLY	406	118.858 49.708 40.737 1.00 16.89	B 0
ATOM	9050	N ILE	407	118. 806 50. 618 38. 691 1. 00 14. 84	B N
ATOM	9051	CA ILE	407	120. 161 51. 144 38. 760 1. 00 13. 37	ВС
ATOM	9052	CB ILE	407	120. 797 51. 192 37. 361 1. 00 11. 30	ВС
ATOM	9053	CG2 ILE	407	122. 039 52. 077 37. 373 1. 00 11. 29	B C B C B C
ATOM	9054	CG1 ILE	407	121. 163 49. 768 36. 936 1. 00 9. 82	B C
ATOM	9055	CD1 ILE	407	121. 237 49. 545 35. 446 1. 00 9. 37	B C
ATOM	9056	C ILE	407	119. 991 52. 546 39. 343 1. 00 15. 02	B C
ATOM	9057	0 ILE	407	119. 236 53. 361 38. 819 1. 00 14. 39	B 0
ATOM	9058	N GLU	408	120.692 52.825 40.431 1.00 16.63 120.552 54.105 41.105 1.00 18.23	B N
ATOM ATOM	9059 9060	CA GLU CB GLU	408		B C B C
ATOM	9061	CB GLU CG GLU	408 408		
ATOM	9062	CG GLU	408	119. 290 52. 815 42. 906 1. 00 23. 80 117. 916 53. 275 42. 456 1. 00 27. 87	B C B C
ATOM	9063	OE1 GLU	408	117. 135 52. 429 41. 967 1. 00 30. 29	В 0
ATOM	9064	OE1 GLU	408	117.612 54.483 42.598 1.00 29.06	B 0
111 0112		225 000	700	111.010 03.300 10.000 1.00 00.00	# U

						(Continued)
					FIG. 4-186	
ATOM	9065	С	GLU	408	121.687 55.094 40.888 1.00 19.22	ВС
ATOM	9066	0	GLU	408	121.468 56.306 40.924 1.00 21.06	B 0
ATOM	9067	N	ALA	409		B N
ATOM	9068	CA	ALA	409		ВС
ATOM	9069	CB	ALA	409		B C
ATOM	9070	C	ALA	409		B C
ATOM	9071	0	ALA	409		B 0
ATOM	9072	N	LEU	410		B N
ATOM ATOM	9073 9074	CA CB	LEU LEU	410 410		B C B C
ATOM	9075	CG	LEU	410	120. 122 54. 517 50. 657 1. 00 10. 00 11 127. 767 54. 292 35. 862 1. 00 18. 12 I	
ATOM	9076		LEU	410		B C
ATOM	9077		LEU	410	127. 144 54. 224 34. 467 1. 00 14. 82	
ATOM	9078	C	LEU	410	128. 356 55. 969 38. 356 1. 00 18. 72	
ATOM	9079	Ō	LEU	410	128. 228 57. 175 38. 190 1. 00 20. 28	
ATOM	9080	N	THR	411	129. 532 55. 396 38. 589 1. 00 18. 37 I	
ATOM	9081	CA	THR	411	130. 786 56. 142 38. 617 1. 00 19. 27 I	
ATOM	9082	CB	THR	411	131. 360 56. 286 40. 060 1. 00 18. 85	
ATOM	9083	0G1		411	131. 869 55. 024 40. 514 1. 00 17. 72	
ATOM	9084		THR	411	130. 284 56. 764 41. 012 1. 00 17. 11 H	
ATOM	9085	C	THR	411	131.744 55.293 37.784 1.00 20.67 H	
ATOM	9086	0	THR	411	131. 374 54. 200 37. 357 1. 00 23. 60 H	
ATOM ATOM	9087 9088	N CA	SER SER	412 412	132. 961 55. 772 37. 543 1. 00 21. 07 H 133. 912 54. 988 36. 753 1. 00 21. 08 H	
ATOM	9089	CB	SER	412	133. 912 54. 988 36. 753 1. 00 21. 08 E 135. 124 55. 827 36. 365 1. 00 18. 37 E	
ATOM	9090	OG	SER	412	135.926 56.086 37.496 1.00 21.11 E	
ATOM	9091	C	SER	412	134. 387 53. 778 37. 548 1. 00 22. 07	
ATOM	9092	ŏ	SER	412	134. 961 52. 843 36. 995 1. 00 23. 13	
ATOM	9093	N	ASP	413	134.144 53.790 38.850 1.00 22.17 E	
ATOM	9094	CA	ASP	413	134. 581 52. 677 39. 673 1. 00 22. 98 E	
ATOM	9095	CB	ASP	413	135. 339 53. 198 40. 895 1. 00 25. 67 E	
ATOM	9096	CG	ASP	413	136. 731 53. 697 40. 548 1. 00 28. 45 E	B C
ATOM	9097		ASP	413	137. 338 54. 395 41. 389 1. 00 31. 52 E	
ATOM	9098		ASP	413	137. 228 53. 385 39. 444 1. 00 29. 95 B	
ATOM	9099	C	ASP	413	133. 446 51. 777 40. 123 1. 00 22. 23 B	
ATOM	9100	0	ASP	413	133. 624 50. 565 40. 248 1. 00 22. 67 B	-
ATOM ATOM	9101 9102	N CA	TYR TYR	414 414	132. 274 52. 362 40. 351 1. 00 21. 41 B 131. 138 51. 575 40. 819 1. 00 18. 45 B	
ATOM	9102	CB	TYR	414	131.138 51.575 40.819 1.00 18.45 B 131.002 51.708 42.329 1.00 15.46 B	
ATOM	9104	CG	TYR	414	132. 101 51. 071 43. 131 1. 00 14. 79 B	
ATOM	9105		TYR	414	132.118 49.699 43.357 1.00 14.59 B	
ATOM	9106		TYR	414	133.093 49.120 44.159 1.00 16.87 B	
ATOM	9107		TYR	414	133.093 51.850 43.718 1.00 14.91 B	
ATOM	9108		TYR	414	134.071 51.282 44.512 1.00 16.48 B	
ATOM	9109	CZ	TYR	414	134.066 49.921 44.733 1.00 16.25 B	
ATOM	9110	OH	TYR	414	135.030 49.369 45.541 1.00 19.68 B	0
ATOM	9111	C	TYR	414	129. 787 51. 898 40. 214 1. 00 17. 91 B	
ATOM	9112	0	TYR	414	129.547 52.990 39.693 1.00 17.06 B	
ATOM	9113	N	LEU	415	128.901 50.917 40.323 1.00 16.46 B	N

ATOM

9162

CG

ASN

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(Continued) FIG. 4-187 ATOM 9114 CA LEU 415 127. 537 51.027 39.855 1.00 14.70 C 127. 297 **ATOM** 9115 CB LEU 415 50.040 38.714 1.00 13.43 C В ATOM 125.924 50.107 Č 9116 CG LEU 415 38.049 1.00 15.02 В 126.044 ATOM 49.620 36.619 9117 CD1 LEU 415 1.00 16.33 В C 124. 899 126. 674 **ATOM** 9118 CD2 LEU 415 49.295 38.852 1.00 15.41 В C ATOM 9119 C LEU 415 50.668 41.066 1.00 15.33 В ATOM 126.777 9120 0 LEU 415 49.566 41.601 1.00 16.82 41.519 125.840 ATOM 9121 N TYR 416 51.5951.00 15.16 В N ATOM 9122 CA TYR 416 124.988 51.313 42.663 1.00 14.80 C В ATOM 124.879 9123 CB TYR 416 52.530 43.566 1.00 13.44 C В 126. 201 127. 031 44. 105 43. 350 **ATOM** 52.997 9124 CG TYR 416 1.00 15.38 В C 53. 835 ATOM 9125 CD1 TYR 416 1.00 14.10 В C ATOM 9126 CE1 TYR 416 128. 240 54.306 43.866 1.00 14.05 $_{\rm C}^{\rm C}$ В 126. 618 127. 823 128. 625 **ATOM** 9127 CD2 TYR 416 52.630 45.386 1.00 14.93 В 9128 ATOM CE2 TYR 416 53.094 45.910 1.00 15.55 C В **ATOM** 9129 CZ TYR 416 53.938 45.147 C 1.00 15.00 B ATOM 9130 OH TYR 416 129.766 54.466 45.699 1.00 14.00 0 B ATOM 9131 C TYR 416 123.604 50.905 42.208 1.00 16.12 C В 123. 041 **ATOM** 51.511 41.296 9132 0 TYR 416 1.00 16.07 В 0 123. 054 121. 730 **ATOM** 9133 TYR N 417 49.878 42.848 1.00 16.79 В N **ATOM** 9134 TYR CA 417 49.407 42.482 1.00 18.72 $_{\rm C}^{\rm C}$ ATOM 9135 CB TYR 121.840 417 48.361 41.365 1.00 20.47 В 122. 456 121. 656 **ATOM** 9136 CG TYR 417 47.039 41.788 1.00 21.65 C В **ATOM** CD1 TYR 9137 417 45.983 42.226 1.00 22.60 $_{\rm C}^{\rm C}$ B ATOM ATOM 9138 CE1 TYR 122.217 417 44.760 42.612 1.00 22.32 B 9139 CD2 TYR 123.835 417 46.843 41.748 1.00 21.40 В C 124. 404 123. 588 ATOM 9140 CE2 TYR 45.626 417 42.135 1.00 21.84 В $_{\rm C}^{\rm C}$ ATOM 9141 CZ TYR 417 44.590 42.565 1.00 22.22 B ATOM ATOM TYR 9142 ОН 417 124.139 43.386 42.950 1.00 22.23 В 0 120. 973 121. 523 9143 C TYR 417 48.824 43.667 1.00 18.97 В C **ATOM** 9144 0 TYR 417 48.640 44.746 1.00 18.94 В 0 **ATOM** N 9145 ILE 418 119.695 48.551 43.453 1.00 19.05 В N ATOM ATOM 9146 CA ILE 418 118.857 47.971 44.485 1.00 20.55 В C 117. 677 116. 692 9147 ILE CB 418 48.906 44.840 1.00 19.77 В C **ATOM** 9148 CG2 ILE 418 48.187 45.742 1.00 20.86 **ATOM** 9149 CG1 ILE 418 118.210 50.148 45.551 1.00 20.46 C ATOM 9150 CD1 ILE 418 117.183 51.211 45.792 1.00 23.81 C B ATOM 118. 337 9151 C ILE 418 46.651 43.947 1.00 20.17 C 9152 9153 **ATOM** 0 ILE 418 118.011 46.546 42.767 1.00 21.74 В 0 ATOM ATOM N SER 419 118. 272 45.642 44.808 1.00 19.61 N C В 117. 798 118. 969 9154 CA SER 419 44.327 44.396 1.00 18.91 B B **ATOM** 9155 CB SER 419 43.923 43.480 1.00 17.21 C 9156 9157 **ATOM** 0G SER 419 . 119.797 43.183 45.030 1.00 19.02 B 0 ATOM ATOM C SER 419 117. 155 43.632 45.578 Č 1.00 18.48 B 9158 0 SER 419 117.216 44.131 46.699 1.00 19.32 B ATOM 9159 N ASN 420 116.536 42.481 45.326 1.00 17.64 В NCCCC ATOM 9160 CA ASN 420 115.913 41.716 46.395 1.00 16.73 В **ATOM** 9161 CB ASN 420 114.448 41.406 1.00 13.22 46.067 В

40.740 SUBSTITUTE SHEET (RULE 26)

44.724

1.00 13.67

114.279

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										(Continued)
					FIC	3. 4-	188			(Continued)
ATOM	9163	OD:	I ASN	420	115.220	40. 146	44. 193	1.00 14.68	В	0
ATOM	9164		2 ASN	420	113.072	40.818	44. 169	1.00 7.98	В	N
ATOM	9165	C	ASN	420	116.700	40. 426	46.638	1.00 16.85	B	Ċ
ATOM	9166	0	ASN	420	116. 135	39.368	46.910	1.00 18.37	B	0
ATOM	9167	N	GLU	421	118.018	40.532	46.543	1.00 17.15	В	N
ATOM	9168	CA	GLU	421	118.895	39. 393	46.754	1.00 19.34	В	C
ATOM	9169	CB	GLU	421	120. 291	39.694	46.195	1.00 18.78	В	· C
ATOM	9170	CG	GLU	421	121.358	38. 747	46.734	1.00 20.75	В	C
ATOM	9171	CD	GLU	421	122.661	38. 782	45.951	1.00 22.48	В	С
ATOM	9172		GLU	421	123.169	39.890	45.661	1.00 21.18	В	0
ATOM	9173		2 GLU	421	123.184	37. 689	45.639	1.00 22.04	В	0
ATOM	9174	C	GLU	421	119.028	38. 945	48. 218	1.00 19.80	В	C
ATOM	9175	0	GLU	421	118.960	37. 756	48.519	1.00 20.89	В	0
ATOM	9176	N	TYR	422	119. 223	39. 897	49. 120	1.00 19.38	В	Ŋ
ATOM	9177	CA	TYR	422	119.401	39. 596	50. 530	1.00 19.16	В	C
ATOM	9178	CB	TYR	422	119.386	40. 895	51.326	1.00 19.06	В	C
ATOM ATOM	9179 9180	CG	TYR TYR	422	119.881	40. 746	52. 741	1.00 21.59	В	C
ATOM	9181		TYR	422 422	121.046 121.510	40. 023	53.024	1.00 19.84	В	C
ATOM	9182		TYR	422	119. 198	39. 893 41. 334	54. 314 53. 798	1.00 19.73	В	C
ATOM	9183		TYR	422	119.658	41. 210	55. 097	1.00 21.32 1.00 23.82	В	C
ATOM	9184	CZ	TYR	422	120.813	40. 488	55. 347	1.00 23.64	B B	C
ATOM	9185	OH	TYR	422	121. 267	40. 376	56. 637	1.00 28.92	В	C 0
ATOM	9186	C	TYR	422	118. 401	38. 600	51.114	1.00 20.84	В	Č
ATOM	9187	ŏ	TYR	422	117.187	38. 779	51.012	1.00 22.40	В	0
ATOM	9188	N	LYS	423	118. 933	37. 546	51.732	1.00 21.52	В	N
ATOM	9189	CA	LYS	423	118. 130	36.486	52.340	1.00 21.53	B	Ĉ
ATOM	9190	CB	LYS	423	117.436	36.995	53.608	1.00 22.83	B	č
ATOM	9191	CG	LYS	423	118.393	37. 278	54.751	1.00 25.85	B	č
ATOM	9192	CD	LYS	423	117.677	37.707	56.020	1.00 27.71	B	č
ATOM	9193	CE	LYS	423	118.692	38.082	57.098	1.00 31.46	B	č
ATOM	9194	NZ	LYS	423	118.052	38.548	58.367	1.00 31.96	В	N
ATOM	9195	C	LYS	423	117.097	35.906	51.378	1.00 21.44	В	C
ATOM	9196	0	LYS	423	116.114	35. 293	51.797	1.00 22.16	В	0
ATOM	9197	N	GLY	424	117. 331	36.106	50.086	1.00 20.50	В	N
ATOM	9198	CA	GLY	424	116.430	35. 595	49.070	1.00 20.06	В	С
ATOM	9199	C	GLY	424	114.969	35.945	49. 274	1.00 20.45	В	C
ATOM	9200	0	GLY	424	114.102	35. 120	49.013	1.00 21.91	В	0
ATOM	9201	N	MET	425	114.695	37. 163	49. 739	1.00 20.34	В	N
ATOM	9202	CA	MET	425	113.322	37. 627	49. 968	1.00 18.53	В	C
ATOM	9203	CB	MET	425	113. 234	38. 329	51.317	1.00 19.68	В	C
ATOM	9204	CG	MET	425 425	113.756	37. 501	52. 469	1.00 22.38	В	C
ATOM ATOM	9205 9206	SD CE	MET	425 425	113.506	38. 352	54.020	1.00 24.27	В	S
ATOM	9200	CE	MET MET	425 425		38.663	53. 907	1.00 21.26	В	C
ATOM	9208	0	MET	425 425		38. 604	48.871	1.00 16.75	В	C
ATOM	9209	N	PRO	425 426		39. 725 38. 206		1.00 17.33	В	0
ATOM	9210	CD	PRO	426		36. 969		1.00 16.64 1.00 17.29	В	N
ATOM	9211	CA	PRO	426		39. 089		1.00 17.29	B B	C C
111 Old	0011	OH	1 1/0	T40	111.000	JJ. UOJ	40. JIV	1.00 10.49	Ŋ	r

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				EIC 4 190	(Continued)
				FIG. 4-189	•
ATOM ATOM	9212 9213	CB PRO	426 426	110. 523 38. 233 46. 140 1. 00 15. 30 B 110. 816 36. 823 46. 561 1. 00 15. 73 B	C C
ATOM	9214	C PRO	426	110.901 40.379 47.416 1.00 15.48 B	C
ATOM	9215	0 PRO	426	110. 913 41. 402 46. 727 1. 00 15. 90 B	ŏ
ATOM	9216	N GLY	427	110. 362 40. 321 48. 630 1. 00 14. 46 B	N
ATOM	9217	CA GLY	427	109. 718 41. 480 49. 217 1. 00 13. 34 B	C
ATOM	9218	C GLY	427	110.649 42.449 49.919 1.00 13.11 B	С
ATOM	9219		427	110. 184 43. 462 50. 452 1. 00 14. 26 B	0
ATOM	9220	N GLY	428	111. 947 42. 144 49. 942 1. 00 9. 68 B	N
ATOM ATOM	9221 9222	CA GLY C GLY	428 428	112.902 43.036 50.577 1.00 8.65 B 113.735 43.771 49.538 1.00 10.35 B	C
ATOM	9223	0 GLY	428	113. 735 43. 771 49. 538 1. 00 10. 35 B 113. 778 43. 363 48. 377 1. 00 10. 03 B	C 0
ATOM	9224	N ARG	429	114.406 44.844 49.946 1.00 11.09 B	N N
ATOM	9225	CA ARG	429	115. 224 45. 630 49. 023 1. 00 12. 98 B	Ċ.
ATOM	9226	CB ARG	429	114. 349 46. 667 48. 314 1. 00 14. 68 B	Č.
ATOM	9227	CG ARG	429	113. 580 46. 084 47. 144 1. 00 18. 95 B	C
ATOM	9228	CD ARG	429	112. 423 46. 947 46. 701 1. 00 18. 69 B	C
ATOM	9229	NE ARG	429	111.590 46.279 45.699 1.00 19.88 B	·N
ATOM ATOM	9230 9231	CZ ARG NH1 ARG	429	111.184 45.008 45.769 1.00 21.09 B	<u>C</u> .
ATOM	9232	NH2 ARG	429 429	111. 535 44. 227 46. 791 1. 00 17. 36 B 110. 390 44. 520 44. 825 1. 00 20. 65 B	N
ATOM	9233	C ARG	429	110. 390 44. 520 44. 825 1. 00 20. 65 B 116. 420 46. 328 49. 678 1. 00 13. 64 B	C .
ATOM	9234	O ARG	429	116. 291 46. 983 50. 707 1. 00 13. 96 B	0
ATOM	9235	N ASN	430	117.584 46.198 49.056 1.00 12.81 B	N
ATOM	9236	CA ASN	430	118. 784 46. 812 49. 585 1. 00 13. 48 B	Ċ
ATOM	9237	CB ASN	430	119. 605 45. 767 50. 344 1. 00 11. 94 B	C
ATOM	9238	CG ASN	430	118. 985 45. 411 51. 677 1. 00 12. 47 B	C
ATOM	9239	OD1 ASN	430	119. 104 46. 167 52. 652 1. 00 11. 56 B	0
ATOM ATOM	9240 9241	ND2 ASN C ASN	430	118. 293 44. 277 51. 727 1. 00 7. 39 B	N
ATOM	9242	0 ASN	430 430	119. 644 47. 477 48. 528 1. 00 14. 50 B 119. 530 47. 189 47. 335 1. 00 14. 26 B	C
ATOM	9243	N LEU	431	119. 530 47. 189 47. 335 1. 00 14. 26 B 120. 504 48. 377 48. 992 1. 00 16. 18 B	O N
ATOM	9244	CA LEU	431	121. 425 49. 107 48. 135 1. 00 17. 01 B	C
ATOM	9245	CB LEU	431	121. 709 50. 496 48. 713 1. 00 16. 67 B	č
ATOM	9246	CG LEU	431	122. 825 51. 279 48. 012 1. 00 18. 10 B	Č
ATOM	9247	CD1 LEU	431	122. 501 51. 399 46. 528 1. 00 17. 30 B	C
ATOM	9248	CD2 LEU	431	122. 998 52. 651 48. 667 1. 00 14. 93 B	C
ATOM ATOM	9249	C LEU	431	122. 729 48. 338 48. 022 1. 00 17. 39 B	C
ATOM	9250 9251	O LEU N TYR	431 432	123. 367 48. 018 49. 028 1. 00 19. 06 B	0
ATOM	9252	CA TYR	432	123. 112 48. 038 46. 789 1. 00 17. 62 B 124. 344 47. 317 46. 511 1. 00 18. 05 B	N
ATOM	9253	CB TYR	432	124. 344 47. 317 46. 511 1. 00 18. 05 B 124. 061 45. 978 45. 826 1. 00 17. 24 B	C C
ATOM	9254	CG TYR	432	123. 334 44. 944 46. 654 1. 00 18. 80 B	C
ATOM	9255	CD1 TYR	432	121. 962 45. 034 46. 883 1. 00 19. 62 B	Č
ATOM	9256	CE1 TYR	432	121. 289 44. 049 47. 601 1. 00 19. 23 B	C
ATOM	9257	CD2 TYR	432	124. 015 43. 843 47. 169 1. 00 17. 63 B	C
ATOM ATOM	9258	CE2 TYR	432	123. 360 42. 862 47. 882 1. 00 18. 49 B	Ç
ATOM	9259 9260	CZ TYR OH TYR	432	121. 996 42. 968 48. 099 1. 00 20. 13 B	C .
VIOU	2200	on 11K	432	121. 358 41. 994 48. 834 1. 00 21. 75 B	0

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						(Continued)
					FIG. 4-190	(CONTINUOU)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	9261 9262 9263 9264 9265 9266 9267 9270 9271 9272 9273 9274 9275	C O N CA CB CC CD CE NZ C O N CA CB CCB CCB CCB CCB CCB CCB CCB CCB C		432 432 433 433 433 433 433 433 434 434	125. 193 48. 142 45. 557 1. 00 17. 78 B 124. 700 49. 066 44. 903 1. 00 18. 57 B 126. 474 47. 805 45. 486 1. 00 16. 13 B 127. 386 48. 460 44. 563 1. 00 14. 57 B 128. 237 49. 536 45. 251 1. 00 16. 46 B 129. 297 49. 022 46. 215 1. 00 16. 27 B 130. 239 50. 146 46. 606 1. 00 16. 51 B 131. 190 49. 723 47. 712 1. 00 16. 69 B 132. 101 50. 834 48. 104 1. 00 17. 27 B 128. 269 47. 343 44. 058 1. 00 13. 68 B 128. 654 46. 454 44. 820 1. 00 11. 44 B 128. 564 47. 364 42. 767 1. 00 13. 85 B 129. 411 46. 331 42. 191 1. 00 15. 56 B 128. 645 45. 504 41. 124 1. 00 14. 45 B 128. 054 46. 429 40. 061 1. 00 11. 95 B	C O N C C C N C O N C C C C
ATOM ATOM	9276 9277	CG1 CD1	ILE	434 434	129. 580 44. 458 40. 518 1. 00 14. 14 B 128. 978 43. 676 39. 379 1. 00 14. 42 B	Č C
ATOM ATOM	9278 9279	C 0	ILE ILE	434 434	130. 646 46. 973 41. 573 1. 00 16. 13 B 130. 554 48. 003 40. 915 1. 00 17. 71 B	C 0
ATOM ATOM	9280 9281	N CA	GLN GLN	435 435	131. 804 46. 374 41. 809 1. 00 18. 33 B 133. 045 46. 907 41. 263 1. 00 20. 88 B	N C
ATOM ATOM	9282 9283	CB CG	GLN GLN	435 435	134. 253 46. 264 41. 956 1. 00 21. 76 B 135. 490 47. 145 41. 958 1. 00 24. 28 B	C C
ATOM	9284	CD	GLN	435	136.715 46.461 42.547 1.00 25.69 B	С
ATOM ATOM	9285 9286	OE1 NE2		435 435	136. 763 46. 154 43. 741 1. 00 26. 08 B 137. 713 46. 220 41. 705 1. 00 24. 68 B	O N
ATOM	9287	C	GLN	435	133.068 46.617 39.767 1.00 20.60 B	C
ATOM ATOM	9288 9289	O N	GLN LEU	435 436	132. 969 45. 465 39. 348 1. 00 20. 57 133. 200 47. 668 38. 965 1. 00 21. 54	0 N
ATOM	9290		LEU	436	133. 200 47. 668 38. 965 1. 00 21. 54 B 133. 197 47. 527 37. 513 1. 00 23. 39 B	N C
ATOM	9291	CB	LEU	436	133.050 48.905 36.880 1.00 21.46 B	č
ATOM	9292	CG	LEU	436	131.785 49.596 37.386 1.00 19.80 B	C C
ATOM	9293	CD1		436	131.748 51.035 36.920 1.00 19.31 B	C
ATOM ATOM	9294 9295	CD2 C	LEU .	436 436	130.572 48.831 36.895 1.00 18.85 B 134.391 46.790 36.908 1.00 25.55 B	C
ATOM	9296	Ö	LEU .	436	134. 391 46. 790 36. 908 1. 00 25. 55 B 134. 294 46. 242 35. 810 1. 00 27. 46 B	C 0
ATOM	9297	Ň	SER	437	135. 517 46. 775 37. 613 1. 00 26. 98 B	N
ATOM	9298	CA	SER	437	136.690 46.069 37.119 1.00 26.89 B	Ĉ
ATOM	9299	CB	SER	437	137. 967 46. 683 37. 689 1. 00 26. 26 B	C
ATOM	9300	0G	SER	437	137. 940 46. 694 39. 102 1. 00 31. 19 B	0
ATOM ATOM	9301 9302	C 0	SER SER	437 437	136.593 44.597 37.507 1.00 27.29 B 137.152 43.736 36.832 1.00 29.17 B	C
ATOM	9303		ASP	438	137.152 43.736 36.832 1.00 29.17 B 135.882 44.310 38.595 1.00 26.66 B	O N
ATOM	9304		ASP	438	135. 704 42. 930 39. 049 1. 00 26. 32 B	C
ATOM	9305	CB	ASP	438	136.702 42.588 40.151 1.00 28.65 B	č
ATOM	9306		ASP	438	136.622 41.135 40.571 1.00 30.81 B	C
ATOM	9307	0D1		438	135. 517 40. 557 40. 495 1. 00 32. 19 B	0
ATOM ATOM	9308 9309	0D2 C	ASP ASP	438	137. 659 40. 575 40. 990 1. 00 33. 46 B	0
UION	3003	U	UOL	438	134. 286 42. 691 39. 572 1. 00 24. 90 B	С

				FIG. 4-191	(Continued)
ATOV	0210	0 ACD	400		D 0
ATOM ATOM	9310 9311	0 ASP N TYR	438 439		B 0
ATOM	9312		439		B N B C
ATOM	9313		439		B C C
ATOM	9314		439		B C
ATOM	9315	CD1 TYR	439		B C
ATOM	9316	CEI TYR	439		B C
ATOM	9317	CD2 TYR	439		B C
ATOM	9318	CE2 TYR	439		B C
ATOM	9319	CZ TYR	439		B C
ATOM	9320	OH TYR	439		B 0
ATOM	9321	C TYR	439		ВС
ATOM	9322	0 TYR	439	130. 882 40. 801 40. 933 1. 00 25. 27	B 0
ATOM	9323	N THR	440	132. 953 40. 030 40. 584 1. 00 24. 21	B N
ATOM	9324	CA THR	440		B C
ATOM	9325	CB THR	440		B C
ATOM	9326	OG1 THR	440		B 0
ATOM	9327	CG2 THR	440		B C
ATOM	9328	C THR	440	132. 712 39. 852 43. 014 1. 00 22. 79	B C
ATOM	9329	0 THR	440		B 0
ATOM ATOM	9330 9331	N LYS CA LYS	441	133. 200 41. 087 43. 039 1. 00 22. 86	B N
ATOM	9332	CA LYS CB LYS	441 441		B C
ATOM	9333	CG LYS	441		B C
ATOM	9334	CD LYS	441		B C B C
ATOM	9335	CE LYS	441		B C B C
ATOM	9336	NZ LYS	441		B N
ATOM	9337	C LYS	441		B C
ATOM	9338	0 LYS	441		B 0
ATOM	9339	N VAL	442		B N
ATOM	9340	CA VAL	442		B C
ATOM	9341	CB VAL	442		B Č
ATOM	9342	CG1 VAL	442		B C
ATOM	9343	CG2 VAL	442		B C
ATOM	9344	C VAL	442		ВС
ATOM	9345	O VAL	442		В 0
ATOM	9346	N THR	443	129. 129 44. 528 47. 066 1. 00 20. 64	
ATOM	9347	CA THR	443		3 C
ATOM	9348	CB THR	443	130.040 46.035 48.801 1.00 24.13	
ATOM	9349	OG1 THR	443	131. 370 45. 566 48. 546 1. 00 28. 90 I	
ATOM	9350	CG2 THR	443	129. 923 46. 442 50. 255 1. 00 22. 91	
ATOM ATOM	9351	C THR	443	127.641 45.475 48.819 1.00 23.06 H	
ATOM	9352 9353	O THR	443	127. 210 46. 483 48. 254 1. 00 26. 29 H	
ATOM	9354	N CYS CA CYS	444	126. 948 44. 835 49. 754 1. 00 21. 88 E	
ATOM	9355	CA CYS C CYS	444	125. 656 45. 368 50. 163 1. 00 22. 22 E	
ATOM	9356	0 CYS	444 444	125. 963 46. 516 51. 115 1. 00 20. 79 E 126. 866 46. 411 51. 941 1. 00 19. 89	_
ATOM	9357	CB CYS	444 444	126. 866 46. 411 51. 941 1. 00 19. 89 E 124. 801 44. 328 50. 878 1. 00 24. 50 E	
ATOM	9358	SG CYS	444	124. 801 44. 328 50. 878 1. 00 24. 50 E	
111 0111		20 010	777	140, 101 44, 300 01, 441 1, 00 41, 44 E	, 9

					FIC	. 4	-192	,		(Continued)
ATOM	9359		LEU	445	125. 205	47. 602	51.005		В	N
ATOM	9360			445	125.442	48.785	51.824		B	Ċ
ATOM	9361	CB		445	125.651	49.988		1.00 15.76	В	C
ATOM	9362	CG		445	126. 714	49. 756	49.812	1.00 15.86	В	C
ATOM ATOM	9363		1 LEU 2 LEU	445	126.930	51.008		1.00 13.93	В	C
ATOM	9364 9365	CD	LEU LEU	445	128.007	49.333	50. 480	1.00 12.34	В	Č .
ATOM	9366	0	LEU	445 445	124. 333 124. 446	49. 099 50. 036	52.814 53.608	1.00 19.64	В	C
ATOM	9367	N	SER	446	123. 262	48. 314	52. 776	1.00 20.41 1.00 21.11	В	0 N
ATOM	9368	CA	SER	446	122. 131	48. 552	53. 656	1.00 21.11	B B	N C
ATOM	9369	CB	SER	446	120. 947	49. 077	52. 834	1.00 20.24	В	C
ATOM	9370	0G	SER	446	120.577	48. 143	51.829	1.00 18.25	В	Õ
ATOM	9371	C	SER	446	121.708	47.307	54. 411	1.00 20.86	B	č
ATOM	9372	0	SER	446	121.085	47.404	55.463	1.00 21.91	В	0
ATOM	9373	N	CYS	447	122. 043	46. 141	53. 874	1.00 21.42	В	N
ATOM	9374	CA	CYS	447	121.667	44.875	54. 495	1.00 23.05	В	C
ATOM ATOM	9375	C	CYS	447	121. 845	44.816	56.004	1.00 23.84	В	С
ATOM	9376 9377	O CB	CYS CYS	447 447	120.881	44.602	56. 739	1.00 24.50	В	0
ATOM	9378	SG	CYS	447	122. 461 122. 134	43. 722 43. 458	53. 874	1.00 24.68	В	<u>C</u> .
ATOM	9379	N	GLU	448	123. 080	45. 011	52. 103 56. 463	1.00 31.64 1.00 23.42	В	S
ATOM	9380	ĊA	GLU	448		44. 913	57. 881	1.00 23.42	B B	N C
ATOM	9381	CB	GLU	448		44. 358	58. 061	1.00 24.37	В	C
ATOM	9382	CG	GLU	448		43.017	57. 395	1.00 28.24	В	Č
ATOM	9383	CD	GLU	448		41.985	57.713	1.00 34.11	В	č
ATOM	9384		GLU	448	123.377	42.073	58.796	1.00 36.48	B	ŏ
ATOM	9385		GLU	448		41.070	56.882	1.00 37.27	В	0
ATOM	9386	C	GLU	448	123. 249	46.162	58. 738	1.00 23.12	В	C
ATOM ATOM	9387 9388	0 N	GLU	448	123. 458	46. 101	59. 948	1.00 24.21	В	0
ATOM	9389	N Ca	LEU LEU	449 449		47. 289	58. 134	1.00 20.81	В	Ŋ
ATOM	9390	CB	LEU	449		48. 516	58. 899	1.00 20.59	В	C
ATOM	9391	CG	LEU	449		49. 592 50. 143	58. 010 56. 909	1.00 18.76	В	<u>C</u> .
ATOM	9392		LEU	449		51.089	56. 045	1.00 17.31 1.00 18.95	В	C
ATOM	9393		LEU	449		50. 868	57. 527	1.00 16.35	B B	C C
ATOM	9394	C	LEU	449		48. 311	60. 144	1.00 22.20	В	C
ATOM	9395	0	LEU	449		48.674	61. 261	1.00 22.97	B	Ŏ
ATOM	9396	N	ASN	450		47. 731	59.937	1.00 22.75	B	N
ATOM	9397	CA	ASN	450			61.011	1.00 21.80	B	Ċ
ATOM	9398	CB	ASN	450			61.344	1.00 23.73	В	Č
ATOM	9399	CG	ASN	450			62.661	1.00 26.67	В	C
ATOM ATOM	9400 9401		ASN	450			63.004	1.00 26.78	В	0
ATOM	9402	C	ASN	450			63. 406	1.00 26.73	В	N
ATOM	9403	0	ASN ASN	450 450			60.469	1.00 22.01	В	C
ATOM	9404	N	PRO	451			60. 072 60. 442	1.00 21.48	В	0
ATOM	9405		PRO	451				1.00 21.65 1.00 20.73	В	N
ATOM	9406		PRO	451				1.00 21.39	B B	C C
ATOM	9407		PRO	451				1.00 19.94	В	C

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							(Continued)
					FIG. 4-193		(Continued)
ATOM	0.400	CC	DDO	451	190 900 42 952 61 900 1 00 91 70	n	0
ATOM ATOM	9408 9409	CG C	PRO PRO	451 451	120. 209 43. 253 61. 290 1. 00 21. 78 117. 035 43. 774 60. 509 1. 00 23. 49	B B	C C
ATOM	9410	0	PRO PRO	451	116.125 43.392 59.774 1.00 25.06	В	0
ATOM	9411	N	GLU	452	116.850 44.003 61.800 1.00 24.25	В	N N
ATOM	9412	CA	GLU	452	115.539 43.793 62.394 1.00 26.56	В	Č
ATOM	9413	CB	GLU	452	115.650 43.767 63.920 1.00 32.21	В	č
ATOM	9414	ĊĠ	GLU	452	116.621 42.720 64.455 1.00 39.54	B	č
ATOM	9415	CD	GLU	452	116.666 42.675 65.976 1.00 44.38	B	Č
ATOM	9416		GLU	452	117. 355 41. 782 66. 521 1. 00 47. 19	В	0
ATOM	9417		GLU	452	116.019 43.529 66.627 1.00 46.89	В	0
· ATOM	9418	C	GLU	452	114.543 44.867 61.968 1.00 25.59	В	С
ATOM	9419	0	GLU	452	113. 374 44. 582 61. 733 1. 00 27. 44	В	0
ATOM	9420	N	ARG	453	115.010 46.101 61.848 1.00 23.36	В	N
ATOM	9421	CA	ARG	453	114.132 47.198 61.478 1.00 21.67	В	C
ATOM	9422	CB	ARG	453	114. 539 48. 463 62. 234 1. 00 21. 94	В	C
ATOM	9423	CG	ARG	453	113. 714 49. 685 61. 872 1. 00 20. 24	В	C
ATOM	9424	CD	ARG	453	111110 001010 021002 1100 11120	. B	C
ATOM	9425	NE C7	ARG	453	113. 364 52. 058 62. 375 1. 00 16. 99	В	N
ATOM	9426 9427	CZ	ARG	453	113. 582 53. 245 62. 927 1. 00 17. 21	В	C
ATOM ATOM	9428		ARG ARG	453 453	114. 579 53. 391 63. 791 1. 00 17. 27 112. 813 54. 280 62. 619 1. 00 14. 66	В	N N
ATOM	9429	C	ARG	453	112. 813 54. 280 62. 619 1. 00 14. 66 114. 077 47. 527 59. 994 1. 00 21. 78	B B	N C
ATOM	9430	Ö	ARG	453	113.024 47.910 59.477 1.00 20.58	В	C 0
ATOM	9431	N	CYS	454	115. 206 47. 368 59. 312 1. 00 21. 64	В	N N
ATOM	9432	CA	CYS	454	115. 293 47. 715 57. 903 1. 00 19. 87	В	C
ATOM	9433	C	CYS	454	115. 598 46. 616 56. 896 1. 00 19. 70	B	č
ATOM	9434	Ö	CYS	454	116.698 46.074 56.865 1.00 21.81	B	ŏ
ATOM	9435	CB	CYS	454	116. 295 48. 847 57. 770 1. 00 19. 47	B	Č
ATOM	9436	SG	CYS	454	115. 666 50. 300 58. 650 1. 00 18. 98	В	Š
ATOM	9437	N	GLN	455	114.608 46.332 56.051 1.00 19.11	В	N
ATOM	9438	CA	GLN	455	114.692 45.305 55.015 1.00 14.77	В	C
ATOM	9439	CB	GLN	455	113.881 44.085 55.457 1.00 13.34	В	C
ATOM	9440	CG	GLN	455	114. 425 43. 413 56. 711 1. 00 12. 92	В	C
ATOM	9441	CD	GLN	455	113. 425 42. 482 57. 387 1. 00 13. 33	В	. C
ATOM	9442	OE1		455	112.514 41.958 56.749 1.00 14.25	В	0
ATOM	9443		GLN	455	113.605 42.266 58.688 1.00 13.47	В	N
ATOM	9444	C	GLN	455	114.156 45.815 53.669 1.00 14.10	В	C
ATOM	9445	0 N	GLN	455	114. 058 45. 059 52. 704 1. 00 14. 35		0
ATOM ATOM	9446	N CA	TYR TYR	456 456	113. 803 47. 094 53. 597 1. 00 13. 95 113. 268 47. 651 52. 355 1. 00 13. 75	В	N
ATOM	9447 9448	CB	TYR	456 456		В	C
ATOM	9449	CG	TYR	456	111. 742 47. 600 52. 387 1. 00 13. 55 111. 049 47. 707 51. 045 1. 00 10. 86	В	C
ATOM	9450		TYR	456	110.504 46.578 50.436 1.00 10.75	B B	C C
ATOM	9451		TYR	456	109.815 46.674 49.236 1.00 9.29	В	Č
ATOM	9452		TYR	456	110.891 48.941 50.405 1.00 9.71	В	Č
ATOM	9453		TYR	456	110. 207 49. 046 49. 200 1. 00 4. 15	В	Č
ATOM	9454	CZ	TYR	456	109.669 47.910 48.629 1.00 8.20	B	č
ATOM	9455	OH	TYR	456	108.949 47.994 47.464 1.00 11.71	В̈́	ŏ
ATOM	9456	C	TYR	456	113.718 49.092 52.190 1.00 14.04	В	C

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					7.10	4	104			(Co	ntinued)
					FIG.	. 4 -	194				
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	9457 9458 9459 9460 9461 • 9462 9463 9464 9465 9466 9467 9468	CE1 CD2	TYR	456 457 457 457 457 457 457 457 457 457	113. 127 114. 752 115. 286 116. 792 117. 271 117. 364 117. 903 117. 714 118. 245 118. 341 118. 877	49. 991 49. 309 50. 646 50. 674 50. 394 49. 088 48. 836 51. 434 51. 193 49. 902 49. 701 51. 192	52. 775 51. 382 51. 152 51. 390 52. 786 53. 275 54. 540 53. 595 54. 850 55. 318 56. 559 49. 742	1. 00 15. 1. 00 15. 1. 00 14. 1. 00 14. 1. 00 14. 1. 00 14. 1. 00 13. 1. 00 13. 1. 00 11. 1. 00 8. 1. 00 15.	11 B 85 B 57 B 62 B 47 B 12 B 34 B 51 B	8 N C C C C C C C C C C C C C C C C C C	
ATOM	9469	Õ	TYR	457	114.827	50. 455	48.797	1.00 17.	46 B	0	
ATOM	9470	N	SER	458		52. 505	49. 624	1.00 14.			
ATOM ATOM	9471 9472	CA CB	SER SER	458 458		53. 207 53. 950	48. 352 48. 163	1.00 14. 1.00 12.			
ATOM	9473	OG	SER	458		55. 138	48. 932	1.00 15.			
ATOM	9474	C	SER	458	116.318	54. 175	48.620	1.00 15.			
ATOM	9475	0	SER	458		54. 431	49.791	1.00 14.			
ATOM ATOM	9476 9477	N CA	VAL VAL	459 459		54. 709 55. 593	47. 574 47. 779	1.00 13. 1.00 13.			
ATOM	9478	CB	VAL	459		54. 853	47. 433	1.00 13.			
ATOM	9479	CG1	VAL	459		54. 578	45.934	1.00 10.			
ATOM	9480		VAL	459		55. 672	47. 878	1.00 13.			
ATOM	9481	C	VAL	459		56. 882	46.969	1.00 14.			
ATOM ATOM	9482 9483	O N	VAL SER	459 460		57. 007 57. 834	46. 021 47. 347	1.00 14.1 1.00 14.1			
ATOM	9484	CA	SER	460		51. 654 59. 106	46.643	1.00 14.			
ATOM	9485	CB	SER	460		50.116	47. 272	1.00 15.			
ATOM	9486	0G	SER	460		61. 333	46.553	1.00 18.			
ATOM	9487	C	SER	460		9. 629	46.693	1.00 15.			
ATOM	9488	0	SER	460		30.040	47. 752	1.00 14.			
ATOM ATOM	9489 9490	N CA	PHE PHE	461 461		59.611	45. 547	1.00 14.9			
ATOM	9491	CB	PHE	461		30. 068 59. 229	45. 469 44. 454	1.00 14.0 1.00 10.1			
ATOM	9492	CG		461	123. 583		44. 885	1.00 10.			
ATOM	9493	CD1	PHE	461		6.832	44. 792	1.00 7.			
ATOM	9494		PHE	461		7. 444	45. 367	1.00 6.		C	
ATOM	9495		PHE	461		55. 509	45. 172	1.00 6.1			
ATOM	9496		PHE	461	125. 105 - 5		45. 752	1.00 6.3			
ATOM ATOM	9497 9498	CZ C	PHE PHE	461 461		55. 153 51. 533	45.653 45.066	1.00 6.9 1.00 16.3			
ATOM	9499	ŏ	PHE	461		32. 076	44. 340	1.00 17.8			
ATOM	9500	Ň	SER	462		32. 170	45. 528	1.00 18.8			
ATOM	9501	CA	SER	462	124.019 6	3. 555	45.155	1.00 20.5	51 B	C	
ATOM	9502	CB	SER	462		64. 137	46.036	1.00 21.9		-	
ATOM	9503	OG C	SER	462		3. 421	45.878	1.00 24.4			
ATOM ATOM	9504 9505	C 0	SER SER	462 462			43. 687 43. 075	1.00 20.6 1.00 21.2		_	
VIOIII	2000	U	OLIK	7U6	124.001 0		*******	1.00 61.6	ע וי	U	

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					FΙ	G. 4	- 197	,			(Co	ntinued)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	9605 9606 9607 9608 9609 9610 9611 9612 9614 9615 9616 9619 9620 9621 9622 9623	O N CA CB CA CC C C C C C C C C C C C C C C	GLY PRO	474 11 475 11 475 11 475 10 475 10 475 10 475 10 475 10 475 10 476 10 476 10 476 10 477 10 477 10 477 10 477 10 477 10 477 10 477 11 477 11	1. 040 2. 149 0. 643 1. 562 9. 353 9. 445 0. 896 9. 012 7. 840 0. 023 9. 770 9. 524 9. 407 9. 422 9. 072 7. 928 7. 940 6. 586 0. 325 1. 516	47. 425 47. 403 46. 446 45. 333 46. 249 44. 807 44. 680 47. 214 47. 392 47. 818 48. 750 50. 140 50. 307 51. 137 52. 519 53. 412 53. 053 54. 009 53. 114 53. 086 52. 819	57. 091 56. 563 57. 913 58. 219 58. 584 59. 068 59. 411 60. 041 60. 331 61. 415 60. 868 59. 656 61. 748 61. 331 62. 563 63. 514 64. 698 62. 775 60. 414 60. 604	1. 00 1. 00	0 16. 48 0 18. 05 0 16. 25 0 17. 27 0 14. 24 0 13. 06 0 14. 77 0 14. 52 0 16. 67 0 12. 63 0 12. 58 0 11. 74 11. 92 10. 87 13. 02 12. 46 12. 47 13. 40 11. 34	B B B B B B B B B B B B B B B B B B B		ntinued)
ATOM ATOM	9625 9626			78 10	9. 931 3. 541	53. 894 54. 283	59. 414 59. 121	1.00	13.58	В	N	
ATOM	9627). 852	54. 510	58. 455	1.00	14. 52 14. 07	В	C	
ATOM	9628	CB P			9. 962	55. 495	57. 705	1.00	13. 81	B B	C C	
ATOM	9629				3. 638	54. 795	57. 702	1.00	14. 19	В	C	
ATOM	9630			78 112	2. 033	55.188	59. 118		15. 11	В	Č	
ATOM	9631				. 892	55.820	60.163		16. 31	B	ŏ	
ATOM	9632				. 197	55.048	58.490		16.04	B	Ň	
ATOM ATOM	9633				. 444	55.621	58. 982	1.00	15.01	В	Ċ	
ATOM	9634 9635		EU 4' EU 4'		. 279	54. 528	59.657		13.83	В	C	
ATOM	9636	CD1 L			675	54.866	60. 179	1.00	12.46	В	C	
ATOM	9637	CD2 LI			. 606 . 268	55. 990 53. 631	61. 189		13. 23	В	Ç	
ATOM	9638		EU 47		. 204	56. 217	60. 813 57. 801		12. 22 14. 97	В	C	
ATOM	9639	0 LI	EU 47		. 395	55. 557	56. 783		15. 80	B B	C 0	
ATOM			YR 48	0 115	. 627	57.468	57.940		15. 76	В	N	
ATOM	9641	CA TY		0 116	. 350	58. 165	56.883		16.51	В	Ċ	
ATOM	9642	CB TY			. 631	59. 471	56.517		18.80	B	č	
ATOM ATOM	9643 9644	CG TY			. 210	59. 293	56.024		20.33	В	C	
ATOM	9645	CE1 TY			910	59. 364	54.664		22. 57	В	С .	
ATOM	9646	CD2 TY			604 170		54. 196	1.00		В	C	
ATOM	9647	CE2 TY	R 48				56. 915 56. 464	1.00		В	C	
ATOM	9648	CZ TY						1.00 1.00		B B	C	
ATOM	9649	OH TY	TR 48					1.00		В	C 0	
ATOM	9650	C TY	R 48	0 117.				1.00		В	C	
ATOM	9651	0 TY	_		910	59. 005	58. 482	1.00	15.89	B	ŏ	
ATOM	9652	N TH	IR 48	l 118.	743	58. 179	56. 559	1.00	15.76	В	N	

(Continued)

										(Cor
					FIG	. 4 -	198			
ATOM	9653	CA	THR	481	120. 129	58. 431	56.924	1.00 15.65	В	C
ATOM	9654	CB	THR	481	120.774	57. 163	57.480	1.00 14.54	В	C
ATOM	9655	0G1	THR	481	120. 459	56.065	56.622	1.00 18.10	В	0
ATOM	9656		THR	481	120. 256	56.864	58.858	1.00 15.87	В	C
ATOM	9657	С	THR	481	120.964	58. 919.	55. 752	1.00 16.24	В	C
ATOM	9658	0	THR	481	120.650	58. 648	54. 602 ·		В	0
ATOM	9659	N	LEU	482	122.035	59.646	56.058	1.00 18.90	В	N
ATOM	9660		LEU	482	122. 937	60. 166	55. 038	1.00 19.21	В	C
ATOM	9661	CB	LEU	482	123. 203	61.653	55. 279	1.00 20.10	В	C
ATOM	9662	CG	LEU	482	123.765	62. 439	54.092	1.00 21.90	В	C
ATOM	9663		LEU	482	122. 736	62. 475	52.975	1.00 21.10	В	C
ATOM	9664		LEU	482	124. 115	63.856	54. 525	1.00 22.66	В	C
ATOM	9665	C	LEU	482	124. 243	59. 373	55. 121	1.00 19.39	В	C
ATOM	9666	0	LEU	482	124.684	59.013	56. 210	1.00 20.79 1.00 18.33	В	O N
ATOM	9667	N	HIS	483	124.849	59. 096 58. 332	53. 970 53. 903	1.00 16.33	B B	C
ATOM	9668	CA	HIS	483	126.090 125.791	56. 894	53. 488	1.00 10.19	В	C
ATOM	9669	CB CG	HIS	483 483	123. 791	56. 245	54. 276	1.00 14.33	В	Č
ATOM	9670 9671		HIS HIS	403 483	123.358	56. 434	54. 264	1.00 14.83	В	Č
ATOM ATOM	9672		HIS	483	124. 933	55. 258	55. 211	1.00 16.09	В	N
ATOM	9673		HIS	483	123. 788	54. 867	55. 736	1.00 13.84	В	Č
ATOM	9674		HIS	483	122.816	55. 565	55. 178	1.00 14.31	В	N
ATOM	9675	C	HIS	483	127.043	58. 939	52. 868	1.00 18.94	B	Ċ
ATOM	9676	ŏ	HIS	483	126.617	59. 665	51.961	1.00 19.56	B	ŏ
ATOM	9677	Ň	SER	484	128. 333	58. 645	53.003	1.00 19.52	B	Ň
ATOM	9678	CA	SER	484	129.318	59. 131	52.040	1.00 21.33	B	C
ATOM	9679	CB	SER	484	130. 520	59. 779	52. 738	1.00 21.77	В	Č
ATOM	9680	0G	SER	484	131.351	58.803	53. 344	1.00 24.25	В	0
ATOM	9681	C	SER	484	129.774	57.907	51.259	1.00 21.22	В	C
ATOM	9682	0	SER	484	129.942	56.827	51.830	1.00 19.26	В	0
ATOM	9683	N	SER	485	129.979	58.076	49.960	1.00 22.12	В	N
ATOM	9684·	CA	SER	485	130. 389	56. 967	49.110	1.00 25.62	В	C
ATOM	9685	CB	SER	485	130.095	57. 301	47.645	1.00 26.28	В	C
ATOM	9686	0G	SER	485	128.715	57. 552	47. 444	1.00 30.40	В	0
ATOM	9687	C	SER	485	131.840	56. 495	49. 221	1.00 26.33	В	C
ATOM	9688	0	SER	485	132.097	55. 300	49. 138	1.00 27.23	В	0
ATOM	9689	N	VAL	486	132. 781	57. 416	49. 407	1.00 28.07	В	N
ATOM	9690	CA	VAL	486	134. 194	57.056	49. 468	1.00 29.41	В	C
ATOM	9691	CB	VAL	486	135. 084	58. 284	49. 798	1.00 30.37	В	Č
ATOM	9692		VAL	486	134. 786	58. 797	51.192	1.00 31.49	В	C
ATOM	9693		VAL	486	136. 553	57. 909	49.665	1.00 30.81	В	C
ATOM	9694	C	VAL	486	134. 507	55. 929	50.442	1.00 30.57	В	C
ATOM	9695	0	VAL	486	135. 269	55.016	50.119	1.00 31.62	В	0
ATOM	9696	N	ASN	487	133. 922	55. 979	51.630	1.00 30.95	В	N
ATOM	9697	CA	ASN	487	134.159	54. 928	52.610	1.00 31.75 1.00 35.87	В	C
ATOM	9698	CB	ASN	487	134.888	55. 498	53. 833	1.00 35.87	В	C
ATOM	9699	CG	ASN	487	136.336	55.868	53. 537	1.00 38.35	B B	C
ATOM	9700		ASN	487 497	136.838	56. 895 55. 026	54. 014 52. 759	1.00 37.49	В	O N
ATOM	9701	אטא	ASN	487	137.019		04. (09 40. (09		ע	14

				FIG	. 4 -	199			(Continued)
ATOM	9702	C A	ASN 487		54. 288	53.048	1.00 30.74	В	С
ATOM	9703		ASN 487		53.486	53. 982	1.00 31.45	В	Ő
ATOM	9704		ASP 488		54. 633	52. 364	1.00 28.68	В	N
ATOM	9705		ASP 488		54. 108	52.707	1.00 26.66	В	Č
ATOM	9706		ASP 488		52.636	52. 313	1.00 27.90	B	č
ATOM	9707		ASP 488		52.440	50.816	1.00 29.72	B	č
ATOM	9708				53. 146	50. 161	1.00 31.30	B	ő
ATOM	9709	0D2 A			51.572	50. 290	1.00 32.18	B	ŏ
ATOM	9710		ASP 488		54. 259	54. 204	1.00 25.72	B	č
ATOM	9711		ASP 488		53.382	54.856	1.00 24.30	В	0
ATOM	9712		LYS 489		55.378	54.754	1.00 25.25	В	N
MOTA	9713	CA I	LYS 489		55.610	56.176	1.00 24.10	В	С
ATOM	9714	CB I	LYS 489	131.607	56.529	56.705	1.00 24.94	В	C
ATOM	9715		LYS 489	131.622	57.898	56.069	1.00 29.19	В	С
ATOM	9716		LYS 489	132.805	58.719	56.560	1.00 33.11	В	C
ATOM	9717		LYS 489		60.133	55.995	1.00 34.94	В	C
ATOM	9718		YS 489		60.959	56.541	1.00 39.70	В	N
ATOM	9719		YS 489		56.216	56. 449	1.00 22.29	В	C
ATOM	9720		YS 489		56.872	55. 585	1.00 20.15	В	0
ATOM	9721		GLY 490		55.968	57.657	1.00 22.04	В	N
ATOM	9722		GLY 490		56. 487	58.067	1.00 20.03	В	С
ATOM	9723		LY 490		57.854	58.676	1.00 20.18	В	С
ATOM	9724		ELY 490		57. 989	59. 769	1.00 20.54	В	0
ATOM	9725		EU 491		58. 876	57.965	1.00 19.44	В	N
ATOM	9726		EU 491		60. 233	58. 440	1.00 19.54	В	C
ATOM	9727		EU 491		61.203	57. 283	1.00 20.53	В	C
ATOM ATOM	9728 9729	CG L CD1 L	EU 491		61.167	56. 242	1.00 18.39	В	C
ATOM	9730	CD2 L			62.089	55.090	1.00 19.23	В	C
ATOM	9731		EU 491		61.577	56.898	1.00 18.31	В	C
ATOM	9732		EU 491		60. 555 60. 780	59. 586 60. 713	1.00 20.91	В	C
ATOM	9733		RG 492		60. 566	59. 316	1.00 22.15 1.00 20.73	В	0
ATOM	9734		RG 492		60. 881	60. 364	1.00 20.73	B B	N
ATOM	9735		RG 492		62. 382	60.644	1.00 20.00	В	C C
ATOM	9736		RG 492		63. 244	59. 568	1.00 20.71	В	C
ATOM	9737		RG 492		64. 698		1.00 20.08	В	C
ATOM	9738		RG 492		64. 888	59. 625	1.00 21.13	В	N
ATOM	9739		RG 492		65. 192	58. 466	1.00 23.12	В	C
ATOM	9740	NH1 A			65. 360	57. 380	1.00 24.47	В	N
ATOM	9741	NH2 A			65. 286	58. 383	1.00 23.72	В	N N
ATOM	9742		RG 492		60. 443	60. 085	1.00 21.47	B	Č
ATOM	9743		RG 492		59.998	58. 983	1.00 21.32	В	Ö
ATOM	9744		AL 493		60. 580	61. 107	1.00 20.97	B	Ň
ATOM	9745		AL 493		60. 211	61.018	1.00 21.38	B	Ċ
ATOM	9746		AL 493		59. 537	62. 325	1.00 22.41	B	č
ATOM	9747	CG1 V	AL 493		59. 215	62. 247	1.00 23.17	B	Č
ATOM	9748	CG2 V			58. 266	62.574	1.00 20.83	B	Č
ATOM	9749		AL 493	119.497	61.456		1.00 21.55	B	Č
ATOM	9750	0 V	AL 493			61.580	1.00 21.85	В	0

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					E I C	. 4.	. 2 0 1	ı		(Continued)
				•			201				
ATOM ATOM	9800 9801		2 LEU LEU	500 500	104. 744 105. 745	56. 763 57. 009			В	C	
ATOM	9802		LEU	500	103. 743	56. 407			В В	C	
ATOM	9803		ASP	501	106. 997	56. 601	67. 131		В	0 N	
ATOM	9804			501	107. 301	55. 392	67. 868		В	C	
ATOM	9805			501	108.793	55. 1-20	67. 844		B	č	
ATOM	9806			501		53.848	68. 556		В	č	
ATOM	9807		1 ASP	501		52. 789	68.164		В	0	
ATOM	9808		2 ASP	501		53. 901	69. 512		В	0	
ATOM ATOM	9809 9810		ASP	501		55. 484	69. 309		В	C	
ATOM	9811		ASP LYS	501 502		54. 520	69. 855		В	0	
ATOM	9812			502		56. 645 56. 819	69. 924 71. 301		В	N	
ATOM	9813		LYS	502		58. 184	71. 834	1.00 31.12 1.00 33.97	B B	C C	
ATOM	9814		LYS	502		58. 484	73. 239	1. 00 35. 56	В	Č	
ATOM	9815	CD	LYS	502		59. 822	73. 766		В	č	
ATOM	9816		LYS	502		60.162	75. 083		В	č	
ATOM	9817		LYS	502		59.098	76. 104		B	N	
ATOM	9818		LYS	502		56.679	71.426	1.00 31.95	В	С	
ATOM	9819		LYS	502		55. 937	72. 276	1.00 33.49	В	0	
ATOM ATOM	9820 9821	N CA	MET MET	503		57. 380	70. 574	1.00 32.49	В	N	
ATOM	9822	CB	MET	503 503		57. 307	70.624	1.00 33.25	В	C	
ATOM	9823	CG	MET	503		58. 342 59. 768	69. 690 70. 131	1.00 35.92	В	C	
ATOM	9824	SD	MET	503		60. 993	69. 105	1.00 42.44 1.00 52.16	B B	C S	
ATOM	9825	CE	MET	503		61.581	70. 243	1.00 50.62	В	S C	
ATOM	9826	C	MET	503		55. 927	70. 279	1.00 31.30	В	Č	
ATOM	9827	0	MET	503		55. 413	70. 954	1.00 31.92	В	0	
ATOM	9828	N	LEU	504		55. 318	69. 238	1.00 30.00	B	Ň	
ATOM	9829	CA	LEU	504	102. 471	53. 993	68.836	1.00 29.48	· B	Ĉ	
ATOM	9830	CB	LEU	504		53. 517	67.624	1.00 28.63	В	С	
ATOM ATOM	9831 9832		LEU	504		53. 477	66. 290	1.00 29.55	В	C	
ATOM	9833		LEU LEU	504 504		54. 750	66. 106	1.00 28.10	В	C	
ATOM	9834	C	LEU	504 504		53. 300 52. 998	65. 143	1.00 27.73	В	C	
ATOM	9835	ŏ	LEU	504		51. 991	69. 986 70. 016	1.00 29.56 1.00 27.71	В	C	
ATOM		Ň		505		53. 291	70. 938	1.00 27.71	B B	0 N	
ATOM	9837	CA	GLN	505		52. 425	72. 096	1.00 31.32	В	N C	
ATOM	9838	CB	GLN	505		2. 915	72.927	1.00 36.96	B	Č .	
ATOM	9839	CG	GLN	505		2.836	72. 200	1.00 42.44	B	Č	
ATOM	9840	CD	GLN	505		1.408	71.996	1.00 43.93	B	č	
ATOM	9841		GLN	505		0.746	72.943	1.00 45.80	В	Ö	
ATOM ATOM	9842 9843		GLN	505		0. 925	70. 758	1.00 45.49	В	N	
ATOM	9844	C 0	GLN	505			72.960	1.00 33.38	В	С	
ATOM	9845	N	GLN ASN	505 506			73.634	1.00 32.77	В .	0	
ATOM	9846	CA	ASN	506			72. 928 73. 694	1.00 32.89	В	N	
ATOM	9847	CB	ASN	506			73. 937	1.00 32.38 1.00 35.05	В	C	
ATOM	9848	CG	ASN	506			74. 629	1.00 35.05	B B	C	
					OLIDOTITICE	0.010		1.00 00.07	ט	U	

·· .					E I C	3. 4 -	202			(Continued)
									_	•
ATOM	9849		ASN ASN	506 506	101.426 101.703	55. 608 56. 796	75. 799 73. 903	1.00 41.09 1.00 39.00	B B	O N
ATOM Atom	9850 9851	C	ASN	506	99. 208	52. 933	72.936	1.00 39.00	В	Č
ATOM	9852	Õ	ASN	506	98. 058	52. 995	73.377	1.00 30.93	В	ŏ
ATOM	9853	Ň	VAL	507	99. 516	52.305	71.803	1.00 26.94	B	N
ATOM	9854	CA	VAL	507	98. 497	51.664	70.974	1.00 25.15	В	C
ATOM	9855	CB	VAL	507	98.456	52.293	69.545	1.00 23.88	В	C
ATOM	9856	CG1		507	97. 287	51.730	68.755	1.00 21.31	В	C
ATOM	9857	CG2		507	98. 344	53. 811	69. 633	1.00 22.11	В	C
ATOM	9858	C	VAL	507	98. 717	50. 164	70.825	1.00 25.62	В	C
ATOM	9859	0	VAL	507	99.838	49.676	70.945	1.00 26.78	В	0 N
MOTA	9860	N	GLN	508 508	97. 639 97. 730	49. 432 47. 992	70. 567 70. 381	1.00 25.89 1.00 25.14	B B	N C
ATOM ATOM	9861 9862	CA CB	GLN GLN	508	96. 486	47. 281	70. 381	1.00 23.14	В	C
ATOM	9863	CG	GLN	508	96. 322	47. 397	72. 422	1.00 29.65	В	č
ATOM	9864	CD	GLN	508	95. 190	46. 543	72.958	1.00 30.81	B	č
ATOM	9865	0E1	GLN	508	95. 208	45.312	72.836	1.00 31.32	B	0
ATOM	9866		GLN	508	94.199	47.190	73.561	1.00 29.92	В	N
ATOM	9867	C	GLN	508	97.869	47. 740	68.899	1.00 23.65	В	C .
ATOM	9868	0	GLN	508	96. 944	47. 277	68. 241	1.00 22.60	В	0
ATOM	9869	N	MET	509	99.046	48.063	68. 385	1.00 23.78	В	N
ATOM	9870	CA	MET	509	99.347	47. 895	66.980	1.00 23.48	В	C
ATOM	9871	CB	MET	509	100.667	48.578	66.655	1.00 23.41 1.00 26.19	В	C
ATOM ATOM	9872 9873	CG SD	MET MET	509 509	100. 586 99. 279	50.070 50.681	66. 782 65. 719	1.00 28.19	B B	C S
ATOM	9874	CE	MET	509	100. 207	50.994	64. 209	1.00 25.78	В	č
ATOM	9875	Č	MET	509	99. 425	46.440	66. 579	1.00 23.44	B	č
ATOM	9876	Ö	MET	509	99.902	45.599	67.343	1.00 24.15	B	0
ATOM	9877	N	PR0	510	98.951	46.121	65.365	1.00 22.69	В	N
ATOM	9878	CD	PR0	510	98.308	47.027	64.395	1.00 22.87	В	С
ATOM	9879	CA	PR0	510	98. 974	44. 751	64.854	1.00 21.97	В	. С
ATOM	9880	CB	PRO	510	97. 987	44.807	63. 701	1.00 22.62	В	C
ATOM	9881	CG	PRO	510	98. 248	46. 171	63. 141	1.00 22.72	В	C
ATOM	9882	C	PRO	510 510	100.381	44. 434	64.379	1.00 21.20	В	C
ATOM ATOM	9883 9884	0 N	PRO SER	510 511	101. 249 100. 605	45. 301 43. 188	64. 353 63. 997	1.00 19.97 1.00 22.07	B B	O N
ATOM	9885	CA	SER	511	101.916	42. 782	63. 521	1.00 23.02	В	Č
ATOM	9886	CB	SER	511	102. 481	41.654	64. 392	1.00 23.03	В	č
ATOM	9887	ÖĞ	SER	511	101.653	40. 500	64. 358	1.00 26.12	B	ő
ATOM	9888	C	SER	511	101.773	42.299	62.094	1.00 23.35	В	Č
ATOM	9889	0	SER	511	100.659	42.168	61.583	1.00 24.92	В	0
ATOM	9890	N	LYS	512	102.906	42.035	61.458	1.00 22.83	В	N
ATOM	9891	CA	LYS	512	102. 916	41.556	60.094	1.00 22.46	В	C
ATOM	9892	CB	LYS	512	103. 490	42.615	59. 168	1.00 21.81	В	C
ATOM	9893	CC	LYS	512	103. 494	42. 209	57. 705	1.00 23.24	В	C
ATOM	9894 9895	CD CE	LYS LYS	512 512	103. 820 103. 824	43. 411 43. 080	56. 851 55. 393	1.00 24.28 1.00 23.13	B B	C C
ATOM ATOM	9896	NZ	LYS	512	103. 824	43.000	55. 595 54. 622	1.00 23.13	В	N N
ATOM	9897	C	LYS	512	104. 160	44. 299	54. 022 59. 993	1.00 24.32	В	Č
111 0111	555.	-	210	0.0	100.174	70. DO	JU. JUU	1.00 22.01	-	•

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					(Continued)
				FIG. 4-203	
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	9898 9899 9900 9901 9902 9903 9904 9905 9906 9910 9911 9912 9913 9914 9915 9916 9917 9918 9919 9920 9921 9922 9923 9924 9925 9928 9929	O LYS N LYS CA LYS CB LYS CC LYS CD LYS NZ LYS C LYS NZ LYS O LYS N LEU CA LEU CD1 LEU CD2 LEU C LEU N ASP CA ASP CB ASP CG ASP OD1 ASP OD2 ASP CA ASP CB ASP CCB ASP CCC ASP	512 513 513 513 513 513 513 514 514 514 514 515 515 515 516 516 516 516 516	FIG. 4 - 203 104.803	
ATOM ATOM	9929 9930	CD2 PHE CE1 PHE	516 516	108. 896 30. 808 52. 176 1. 00 22. 68 B 107. 678 29. 042 51. 119 1. 00 21. 58 B 109. 836 29. 885 52. 642 1. 00 21. 89 B	
ATOM ATOM ATOM ATOM	9931 9932 9933 9934	CE2 PHE CZ PHE C PHE O PHE	516 516 516 516	108.609 28.113 51.579 1.00 21.19 B 109.689 28.536 52.342 1.00 20.70 B 104.955 30.117 51.954 1.00 26.95 B 105.063 29.452 52.980 1.00 28.94 B	C C C O
ATOM ATOM ATOM ATOM	9935 9936 9937 9938	N ILE CA ILE CB ILE CG2 ILE	517 517 517 517	104. 307 29. 707 50. 872 1.00 27. 35 B 103. 697 28. 398 50. 755 1.00 28. 12 B 102. 155 28. 470 50. 729 1.00 26. 53 B 101. 645 29. 073 52. 016 1.00 27. 39 B	N C C C
ATOM ATOM ATOM ATOM ATOM	9939 9940 9941 9942 9943	CG1 ILE CD1 ILE C ILE O ILE N ILE	517 517 517 517 518	101. 682 29. 296 49. 537 1. 00 27. 43 B 100. 175 29. 486 49. 486 1. 00 26. 37 B 104. 202 27. 896 49. 411 1. 00 30. 13 B 104. 575 28. 697 48. 551 1. 00 29. 21 B 104. 239 26. 581 49. 228 1. 00 33. 16 B	C C C O N
ATOM ATOM ATOM	9944 9945 9946	CA ILE CB ILE CG2 ILE	518 518 518	104. 709 26. 029 47. 969 1. 00 36. 01 B 105. 680 24. 867 48. 190 1. 00 36. 84 B 106. 133 24. 311 46. 845 1. 00 36. 94 B	C C C

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(Continued)

					FIC	3. 4 -	204			(Contin	iuea)
ATOM ATOM	9947 9948		ILE ILE	518 518	106. 884 107. 976	25. 349 24. 296	49. 000 49. 169	1.00 38.21 1.00 40.77		C	
ATOM	9949	C	ILE	518	103.558	25. 534	47.114	1.00 37.38		Č	
ATOM	9950	0	ILE	518	102.581	25.000	47.624	1.00 38.97	В	0	
ATOM	9951	N	LEU	519	103. 679	25.730	45.808	1.00 39.11		N	
ATOM	9952	CA	LEU	519	102.663	25. 294	44.863	1.00 40.68		C	
ATOM	9953	CB	LEU	519	101.753	26.461	44. 474	1.00 39.71		C	
ATOM	9954	CC	LEU	519	100. 989 100. 051	27. 144 28. 205	45. 612 45. 045	1.00 39.82 1.00 39.14		C C	
ATOM ATOM	9955 9956		LEU LEU	519 519	100.031	26. 107	46. 381	1.00 39.14		Č	
ATOM	9957	CDZ	LEU	519	103. 388	24. 763	43.637	1.00 42.22		Č	
ATOM	9958	ŏ	LEU	519	104. 028	25. 524	42.910	1.00 42.60		Ŏ	
ATOM	9959	N	ASN	520	103. 299	23. 453	43.419	1.00 43.53		N	
ATOM	9960	CA	ASN	520	103. 963	22. 824	42.285	1.00 44.57		C	
ATOM	9961	CB	ASN	520	103. 385	23. 337	40.964	1.00 46.39		C	
ATOM	9962	CG	ASN	520	102.045	22. 726	40.639	1.00 48.97		C	
ATOM	9963 9964		ASN ASN	520 520	101.168 101.871	22. 634 22. 312	41.498 39.386	1.00 50.54 1.00 50.46		O N	
ATOM ATOM	9965	C	ASN	520 520	105. 452	23. 114	42.316	1.00 30.40		C	
ATOM	9966	ő	ASN	520	106. 004	23. 637	41.348	1.00 44.64		Ö	
ATOM	9967	Ň	GLU	521	106.097	22. 791	43. 431	1.00 44.10		N	
ATOM	9968	CA	GLU	521	107. 536	23.012	43.562	1.00 45.15		C	
ATOM	9969	CB	GLU	521	108. 272	22. 387	42. 368	1.00 49.07		С	
ATOM	9970	CG	GLU	521	109. 775	22. 642	42.339	1.00 54.49		C	
ATOM	9971	CD	GLU	521	110.401	22. 274	41.004	1.00 58.04		C	
ATOM ATOM	9972 9973		GLU GLU	521 521	110. 307 110. 986	21. 091 23. 176	40. 597 40. 361	1.00 59.07 1.00 59.78		0 0	
ATOM	9974	C	GLU	521	107. 922	24. 486	43.661	1.00 33.18		C	
ATOM	9975	ŏ	GLU	521	109.034	24. 810	44.072	1.00 42.85		ŏ	
ATOM	9976	N	THR	522	107.014	25. 378	43. 283	1.00 38.59		Ň	
ATOM	9977	CA	THR	522	107.314	26.800	43. 333	1.00 34.63		C	
ATOM	9978	CB	THR	522	106.605	27. 566	42. 198	1.00 34.21	В	C	
ATOM	9979	0G1		522	107. 109	27. 115	40. 936	1.00 34.20		0	
ATOM	9980 9981	CGZ	THR THR	522 522	106.866	29. 057 27. 441	42.318	1.00 33.69 1.00 32.83		C	
ATOM ATOM	9982	0	THR	522 522	106. 959 106. 028	27. 027	44.664 45.350	1.00 32.83		C 0	
ATOM	9983	N	LYS	523	107. 727	28. 464	45.011	1.00 32.10		N	
ATOM	9984	CA	LYS	523	107. 559	29. 206	46. 245	1.00 29.30	B	Ċ	
ATOM	9985	CB	LYS	523	108.940	29.490	46.838	1.00 29.00	В	Č	
ATOM	9986	CG	LYS	523	108. 934	30. 329	48.089	1.00 31.42	В	C	
ATOM	9987	CD	LYS	523	110. 344	30. 567	48.607	1.00 32.07	В	C	
ATOM	9988	CE	LYS	523	111.045	29. 265	48. 943	1.00 33.13	В	Ç	
ATOM	9989	NZ C	LYS LYS	523	112.388	29. 512	49. 545 45. 984	1.00 35.72 1.00 28.56	В	N	
ATOM ATOM	9990 9991	0	LYS	523 523	106. 819 107. 256	30. 519 31. 335	45. 173	1.00 28.36	B B	C 0	
ATOM	9992	N	PHE	524	105. 692	30. 711	46. 661	1.00 25.40	В	Ŋ	
ATOM	9993	CA	PHE	524	104. 912	31. 934	46. 517	1.00 22.61	В	C -	
ATOM	9994	CB	PHE	524	103. 529	31.637	45. 929	1.00 22.69	B	č	
ATOM	9995	CG	PHE	524	103.565	31. 136	44.516	1.00 21.75	В	С	

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				•	FI(G. 4-	206			
	10015	^	L mm	=00	100 451	00.045	E0 500	1 00 01 07	_	•
ATOM	10045	0	MET	528	100. 471	39. 845	58. 720	1.00 21.07	В	0
ATOM	10046	N	ILE	529	98. 432	40. 554	58. 100	1.00 19.01	В	N
ATOM	10047	CA	ILE	529	98. 428	41.614	59. 082	1.00 18.89	В	C
ATOM	10048	CB	ILE	529	97. 718	42. 860	58. 540	1.00 16.80	В	C
ATOM	10049		ILE	529	97.656	43. 937	59.615	1.00 13.98	В	C C C
ATOM	10050		ILE	529	98. 469	43. 368	57. 296	1.00 15.06	.B	C
ATOM	10051		ILE	529	99. 934	43. 701	57. 537	1.00 11.03	В	C
ATOM	10052	C	ILE	529	97. 656	40. 969	60. 225	1.00 20.15	В	C
ATOM	10053	0	ILE	529	96.457	40. 720	60. 124	1.00 20.94	В	0
ATOM	10054	N	LEU	530	98. 359	40.653	61.302	1.00 21.19	В	N
ATOM	10055	CA	LEU	530	97.717	39. 985	62. 420	1.00 21.61	В	C
ATOM	10056	CB	LEU	530	98. 649	38. 907	62. 976	1.00 19.85	В	C
ATOM	10057		LEU	530	99.086	37. 875	61.931	1.00 19.34	В	C
ATOM	10058		LEU	530	100. 238	37. 027	62. 461	1.00 20.33	В	C C C
ATOM	10059		LEU	530	97. 897	37.010	61.562	1.00 19.04	В	C
ATOM	10060	C	LEU	530	97. 294	40.930	63. 521	1.00 22.34	В	C
ATOM	10061	0 N	LEU	530	98.006	41.878	63. 854	1.00 23.45	В	0
ATOM	10062	V.	PRO	531	96.104	40.697	64. 088 63. 711	1.00 23.19 1.00 22.71	В	N
ATOM	10063	CD CA	PRO	531 531	95. 105 95. 600	39. 684 41. 545			В	C
ATOM ATOM	10064 10065		PRO PRO	531	94.188		65. 169 65. 404	1.00 24.33 1.00 22.74	В	C
ATOM	10066	CB CG	PRO	531	94. 166	39.588	64. 967	1.00 22.74	В	C
ATOM	10067	C	PRO	531	96. 490	41. 438	66.407	1.00 25.03	B B	C C
ATOM	10068	0	PRO	531	97. 244	40.478	66. 562	1.00 23.16	В	Ö
ATOM	10069	N	PRO	532	96. 424	42. 433	67. 300	1.00 24.04	В	N N
ATOM	10003	CD	PRO	532	95. 502	43. 581	67. 326	1.00 25.36	В	C
ATOM	10070	CA	PRO	532	97. 246	42. 397	68. 513	1.00 23.30	В	Č
ATOM	10071	CB	PRO	532	96. 868	43. 698	69. 216	1.00 27.08	В	Č
ATOM	10073	CG	PRO	532	95. 443	43.897	68. 793	1.00 26.25	В	Č
ATOM	10074	C	PRO	532	96. 945	41.160	69. 369	1.00 20.25	В	Č
ATOM	10075	ŏ	PRO	532	95. 865	40.579	69. 279	1.00 29.62	В	Ö
ATOM	10076	N	HIS	533	97. 909	40.756	70. 187	1.00 20.65	В	N N
ATOM	10077	CA	HIS	533	97. 738	39.602	71.061	1.00 31.99	B	Ċ
ATOM	10078	CB	HIS	533	96. 749	39. 945	72. 172	1.00 32.50	B	č
ATOM	10079	ĊĞ	HIS	533	96. 981	41. 293	72. 783	1.00 35.12	В	č
		CD2		533		42.370		1.00 36.18	В	č
ATOM	10081		HIS	533	98. 181	41.653	73. 358	1.00 35.49	B	Ň
ATOM	10082		HIS	533	98. 096	42.892	73. 807	1.00 36.37	B	Ċ
ATOM	10083		HIS	533	96. 885	43. 350	73. 544	1.00 37.01	B	Ň
ATOM	10084	C	HIS	533	97. 249	38. 382	70. 286	1. 00 33. 21	В	Ċ
ATOM	10085	Ŏ	HIS	533	96. 447	37. 590	70. 791	1.00 32.78	B	ŏ
ATOM	10086	Ň	PHE	534	97. 739	38. 243	69. 058	1.00 33.50	B	Ň
ATOM	10087	CA	PHE	534	97. 374	37. 125	68. 200	1.00 34.63	B	Ċ
ATOM	10088	CB	PHE	534	98. 283	37. 085	66. 970	1.00 32.35	B	č
ATOM	10089	CG	PHE	534	97. 997	35. 942	66.041	1.00 32.06	B	č
ATOM	10090	CD1		534	96. 790	35. 871	65.354	1.00 32.10	B	č
ATOM	10091		PHE	534	98. 936	34. 938	65.848	1.00 32.66	B	č
ATOM	10092	CE1		534	96. 522	34. 819	64.486	1.00 31.59	B	č
ATOM	10093		PHE	534	98.679	33.879	64.982	1.00 32.91	В	Č

							(Comtinued)
					FIG. 4-207		(Continued)
ATOU	10004	מים	יווזת	E0.4		n	0
ATOM ATOM	10094		PHE PHE	534 534	97. 469 33. 820 64. 298 1. 00 32. 93	В	C
ATOM	10095 10096		PHE	534	97.503 35.806 68.941 1.00 36.77 98.532 35.534 69.565 1.00 37.84	B B	C
ATOM	10090	N	ASP	535	96. 463 34. 982 68. 868 1. 00 39. 07	В	O N
ATOM	10098	CA	ASP	535	96. 480 33. 680 69. 523 1. 00 40. 37	В	C
ATOM	10090	CB	ASP	535	95. 458 33. 639 70. 655 1. 00 42. 55	В	C
ATOM	10100	CG	ASP	535	95.544 32.363 71.465 1.00 45.66	В	Č
ATOM	10101		ASP	535	94. 783 32. 227 72. 445 1. 00 49. 45	В	ŏ
ATOM	10102		ASP	535	96.372 31.494 71.125 1.00 46.59	В	ŏ
ATOM	10103	C	ASP	535	96.159 32.601 68.503 1.00 39.36	B	Č
ATOM	10104	0	ASP	535	95.047 32.540 67.996 1.00 39.17	В	0
ATOM	10105	N	LYS	536	97. 135 31. 746 68. 216 1. 00 40. 23	В	N
ATOM	10106	CA	LYS	536	96.964 30.680 67.233 1.00 41.20	В	С
ATOM	10107	CB	LYS	536	98. 302 30. 001 66. 947 1. 00 42. 62	В	С
ATOM	10108	CG	LYS	536	98. 266 29. 089 65. 731 1. 00 46. 75	В	C
ATOM	10109	CD	LYS	536	99.657 28.577 65.355 1.00 49.06	В	C
ATOM	10110	CE	LYS	536	99. 624 27. 800 64. 040 1. 00 48. 68	В	C
ATOM	10111	NZ	LYS	536	98. 648 26. 676 64. 079 1. 00 48. 77	В	N
ATOM	10112	C	LYS	536	95. 937 29. 620 67. 607 1. 00 40. 95	В	C
ATOM	10113	0	LYS	536	95. 577 28. 785 66. 778 1. 00 41. 99	В	0
ATOM ATOM	10114 10115	N CA	SER SER	537 537	95.464 29.649 68.848 1.00 40.73	В	N
ATOM	10116	CB	SER	537	94. 469 28. 681 69. 296 1. 00 40. 33 94. 598 28. 438 70. 805 1. 00 40. 23	В	C
ATOM	10117	OG	SER	537		В	C
ATOM	10118	C	SER	537	94. 434 29. 636 71. 541 1. 00 40. 12 93. 064 29. 179 68. 968 1. 00 40. 20	В	0
ATOM	10119	ŏ	SER	537	92.103 28.412 68.977 1.00 40.87	B B	C 0
ATOM	10120	Ň	LYS	538	92. 951 30. 469 68. 674 1. 00 39. 23	В	N
ATOM	10121	CA	LYS	538	91.666 31.067 68.337 1.00 37.32	B	C
ATOM	10122	CB	LYS	538	91.629 32.517 68.817 1.00 39.07	В	č
ATOM	10123	CG	LYS	538	92. 298 32. 747 70. 170 1. 00 41. 74	B	č
ATOM	10124	CD	LYS	538	91.534 32.100 71.316 1.00 44.86	B	č
ATOM	10125	CE	LYS	538	90.186 32.773 71.540 1.00 46.82	B	Č
ATOM	10126	NZ	LYS	538	89. 417 32. 121 72. 636 1. 00 47. 36	B	N
ATOM	10127	C	LYS	538	91.507 31.028 66.819 1.00 35.00	В	С
ATOM	10128	0	LYS.	538	92.464 30.754 66.101 1.00 34.33	В	0
ATOM	10129	N	LYS	539	90. 299 31. 288 66. 335 1. 00 33. 57	В	N
ATOM	10130	CA	LYS	539	90. 038 31. 302 64. 895 1. 00 32. 92	В	C
ATOM	10131	CB	LYS	539	89.049 30.197 64.510 1.00 32.99	В	С
ATOM	10132	CG	LYS	539	89.736 28.887 64.143 1.00 36.07	В	C
ATOM	10133	CD	LYS	539	88. 757 27. 739 63. 893 1. 00 39. 32	В	C
ATOM	10134	· CE	LYS	539	87. 720 28. 059 62. 816 1. 00 39. 62	В	C
ATOM ATOM	10135 10136	NZ C	LYS LYS	539 539	86.644 28.969 63.310 1.00 39.49	В	N
ATOM	10130	Ö	LYS	539 539	89.504 32.666 64.471 1.00 31.07	В	C
ATOM	10138	N	TYR	540	88. 424 33. 087 64. 902 1. 00 30. 44 90. 274 33. 356 63. 633 1. 00 27. 48	В	0
ATOM	10139	CA	TYR	540	90. 274 33. 356 63. 633 1. 00 27. 48 89. 893 34. 682 63. 165 1. 00 24. 82	В	N
ATOM	10140	CB	TYR	540	91.096 35.624 63.178 1.00 23.82	В	C
ATOM	10141	CG	TYR	540	91.849 35.702 64.482 1.00 23.61	B B	C C
ATOM	10142	CD1		540	92.614 34.627 64.936 1.00 21.98	В	C
						U	v

											(Continued)
					FIG.	4 -	208				(Continued)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	10179 10180	CD1 CD2 C	TYR TYR TYR TYR PRO PRO PRO PRO PRO LEU	541 541 541 542 542 542 542 543 543 544 544 544 544 544 544 544 544	93. 321 34 91. 810 36 92. 507 36 93. 261 35 93. 950 35 89. 335 34 89. 670 36 87. 820 36 87. 917 35 86. 770 36 87. 243 37 89. 077 36 89. 028 36 90. 133 36 91. 027 35 92. 215 35 93. 296 34 91. 741 35 88. 720 37 90. 368 38 90. 075 39 88. 720 37 90. 368 38 90. 075 39 81. 640 89. 568 41 88. 317 41 89. 409 43 91. 273 39 92. 349 39 91. 091 38 92. 191 38 92. 191 38 92. 191 38 92. 191 38 92. 191 38 92. 191 38 92. 191 38 92. 191 38 92. 191 38 92. 191 38	. 708 . 863 . 955 . 875 . 965 . 694 . 842 . 660 . 667 . 719 . 717 . 629 . 266 . 799 . 147 . 655 . 483 . 768 . 775 . 458 . 872 . 892 . 892 . 892 . 893 . 893	66. 130 65. 257 66. 449 66. 881 68. 062 61. 749 60. 925 61. 452 62. 320 60. 095 60. 228 61. 317 59. 276 59. 841 57. 169 56. 741 55. 816 56. 025 54. 374 55. 954 55. 015 53. 886 53. 113 54. 454 53. 620 53. 966 52. 428 50. 679 49. 819	1.00 1.00	22. 87 22. 87 23. 97 23. 93 21. 22 20. 52 20. 36 19. 90 19. 38 11. 89 11. 89 11. 89 11. 89 11. 89 11. 89 11. 89 11. 87 11. 87 11. 87 11. 87 11. 87 11. 87 11. 87 11. 89 11. 87 11. 87	B B B B B B B B B B B B B B B B B B B	(Continued) C C C C C C C C C C C C C C C C C C
ATOM ATOM ATOM	10180 10181 10182	O N CA	LEU ASP ASP	544 545 545	93. 280 40). 374). 925). 186	49. 819 50. 997 50. 306	1.00 1.00 1.00	15.13	В В В	O N C
ATOM ATOM ATOM	10183 10184 10185	CB CG OD1	ASP ASP ASP	545 545 545	94. 479 43 94. 703 44 94. 285 44	. 069 . 434 . 641	51.117 50.483 49.324	1.00 1.00 1.00	15.71 15.88 14.36	B B B	C C 0
ATOM ATOM ATOM ATOM	10186 10187 10188 10189	OD2 C O N	ASP ASP VAL	545 545 545 546	94. 175 41 95. 235 41 93. 567 42	. 304 . 757 . 135 . 098	51.144 49.004 49.014 47.881	1.00 1.00 1.00 1.00	14.61 13.17 15.03	B B B	0 C 0 N
ATOM ATOM	10190 10191	CA CB	VAL VAL	546 546		. 667 . 579	46.614 46.014	1.00		B B	C C

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					E I C		200			(Continued)
					FIG	r. 4 -	209			
ለጥባህ	10109	CC	I VAL	EAC	09 717	40 194	44 CA7	1 00 17 07	D	C
ATOM ATOM	10192 10193		VAL VAL	546 546	93.717	40. 124 39. 410	44. 647 46. 983	1.00 17.87	В	C
ATOM			VAL		93.109	42. 722		1.00 20.93	В	C
ATOM		0	VAL	546 546	94. 343 93. 601	43. 694	45. 542 45. 447	1.00 17.09	В	C
ATOM	10196		TYR	547	95. 391	42. 519	44. 745	1.00 18.12	В	0
ATOM	10190	CA	TYR	547	95. 591 95. 670	43. 378	43. 595	1.00 15.70 1.00 14.90	В	N C
ATOM	10198	CB	TYR	547	96. 838	44. 335	43. 821	1.00 14.90	B B	C C
ATOM	10199	CG	TYR	547	97. 008	45. 241	42. 622	1.00 12.30	В	C
ATOM	10200		TYR	547	98. 064	45. 063	41.727	1.00 12.04	В	C
ATOM	10200	CF	TYR	547	98. 165	45. 839	40. 578	1.00 12.01	В	C
ATOM	10201		2 TYR	547	96. 057	46. 226	42. 331	1.00 3.37	В	C
ATOM	10203	CE		547	96. 149	47. 002	41. 183	1.00 11.62	В	Č
ATOM	10204	CZ	TYR	547	97. 204	46. 804	40. 314	1.00 10.60	В	Č
ATOM	10205	OH	TYR	547		47. 573	39.179	1.00 12.10	В	ő
ATOM	10206	Č	TYR	547		42. 392	42.485	1.00 13.60	В	č
ATOM	10207	Ŏ	TYR	547	95. 244	42. 205	41.548	1.00 13.39	В	ŏ
ATOM	10208	N	ALA	548		41.763	42.608	1.00 13.66	B	N
ATOM	10209	CA	ALA	548		40.730	41.672	1.00 14.14	B	Ċ
ATOM	10210	CB	ALA	548		39.518	41.807	1.00 11.57	B	č
ATOM	10211	C	ALA	548		41.105	40.207	1.00 13.67	\tilde{B}	č
ATOM	10212	0	ALA	548		40. 234	39.340	1.00 14.21	B	0
ATOM	10213	N	GLY	549	97. 905	42.386	39.913	1.00 13.87	В	N
ATOM	10214	CA	GLY	549	98. 078	42.765	38. 524	1.00 12.26	В	С
ATOM	10215	C	GLY	549	99. 405	42.209	38.046	1.00 12.16	В	C
ATOM	10216	0	GLY	549		41.717	38.855	1.00 12.33	В	0
ATOM	10217	N	PRO	550		42. 256	36.739	1.00 13.98	В	N
ATOM	10218	CD	PRO	550		42.760	35.644	1.00 12.99	В	C
ATOM	10219	CA	PRO	550		41.736	36. 217	1.00 13.32	В	C
ATOM	10220	CB	PRO	550		42.007	34. 721	1.00 14.56	В	С
ATOM	10221	CG	PRO	550		42.015	34. 473	1.00 14.10	В	С
ATOM	10222	C	PRO	550		42.459	36.832	1.00 13.86	В	C
ATOM	10223	0	PRO	550		43. 683	36. 785	1.00 13.45	. В	0
ATOM	10224	N	CYS	551		41.694	37. 405	1.00 14.79	В	N
ATOM ATOM	10225 10226	CA	CYS	551		42. 244	38. 027	1.00 15.51	В	C
ATOM	10227	CB SG	CYS CYS	551		43. 139	37. 036	1.00 17.05	В	C
ATOM	10227	C	CYS	551		43. 567	37. 543	1.00 17.09	В	S
ATOM	10229		CYS	551		43. 018	39. 312	1.00 16.05	В	C
ATOM	10223	O N	SER	551 552		43. 938	39. 702	1.00 15.36	В	0
ATOM	10231	CA	SER	552 552		42. 631 43. 268	39.976	1.00 15.15 1.00 14.65	В	N
ATOM	10232	CB	SER	552			41. 229		В	C .
ATOM	10232	OG	SER	552		43. 149 41. 789	41. 425 41. 427	1.00 14.47	В	C
ATOM	10234	C	SER	552		42.608	42. 418	1.00 14.39 1.00 15.21	B B	0
ATOM	10235	Õ	SER	552		42.006 41.585	42. 273	1.00 15.21	В	C
ATOM	10236	N	GLN	553		43. 201	43. 594	1.00 15.34	В	0 N
ATOM	10237	CA	GLN	553		43. 201 42. 647	44. 794	1.00 14.73	В	C
ATOM	10238	CB	GLN	553			44. 892	1.00 14.31	В	C
ATOM	10239	CG	GLN	553				1.00 15.21	В	C
ATOM	10240	CD	GLN	553				1.00 15.66	В	C
			J. 1	000	OUDOTITUTE			1.00 10.00	n	v

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ATOM

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(Continued) FIG. 4-210 1.00 16.56 0 43.686 46.400 107.812 ATOM 10241 OE1 GLN 553 108.138 41.556 N 45.773 1.00 15.50 В NE2 GLN ATOM 10242 553 C 43.166 1.00 14.58 В 102.921 46.012 ATOM 10243 C GLN 553 1.00 14.77 В 0 44. 295 46.434 0 103.148 ATOM 10244 GLN 553 46.568 1.00 14.78 В N 42.344 102.031 ATOM 10245 N LYS 554 1.00 16.57 В C 42.734 10246 CA LYS 554 101.284 47.754 ATOM C 99.817 42.318 47.633 1.00 17.81 LYS 554 ATOM 10247 CB LYS 99.031 43.142 46.630 1.00 18.63 В ATOM 10248 CG 554 1.00 18.55 99.047 44.612 47.000 В LYS ATOM 10249 CD 554 C В 98.228 44.902 48.261 1.00 18.33 10250 LYS 554 ATOM CE 96.769 44.771 48.035 1.00 13.33 В N LYS ATOM 10251 NZ 554 101.890 42.148 1.00 16.05 В C 49.024 LYS **ATOM** 10252 C 554 42.429 1.00 17.37 В 0 101.424 50.124 10253 LYS ATOM 0 554 10254 10255 В N 102.939 41.350 48.866 1.00 15.91 ALA ATOM N 555 В C 103.622 40.730 50.004 1.00 15.84 ATOM CA ALA 555 39.210 49.833 В C 103.656 1.00 15.51 ATOM 10256 CB ALA 555 В C 41.246 50.142 1.00 14.91 105.041 ATOM 10257 C ALA 555 105.954 40.691 49.539 1.00 15.57 В 0 10258 **ATOM** 0 ALA 555 42.304 50.924 1.00 16.20 В N 105.233 **ATOM** 10259 N **ASP** 556 C 42.854 51.134 1.00 16.65 В 106.571 ATOM 10260 CA ASP 556 C 44.085 50.243 1.00 17.94 В 106.801 ATOM 10261 CB **ASP** 556 50.430 1.00 19.95 C 105.750 45.159 В ATOM 10262 CG ASP 556 105. 355 105. 327 45.429 51.583 1.00 22.16 В 0 **ATOM** 10263 OD1 ASP 556 45. 751 1.00 21.01 В 49.415 0 **ATOM** 10264 OD2 ASP 556 106.862 43.202 52.597 1.00 16.87 В .C **ATOM** 10265 C ASP 556 106.046 42.962 53.480 1.00 15.15 В 0 ATOM 10266 0 ASP 556 108.039 52.847 1.00 17.93 В N ATOM 10267 N THR 557 43.762 108.443 44.132 54.200 1.00 18.07 B C ATOM 10268 CA THR 557 54.396 10269 109.923 43.826 1.00 18.59 В C ATOM CB THR 557 110.687 10270 44.589 53.454 1.00 20.98 В 0 ATOM 0G1 THR 557 C 110.188 42.358 54.157 1.00 19.55 В ATOM 10271 CG2 THR 557 C 108.203 45.616 54.531 1.00 17.89 В ATOM 10272 C THR 557 108.776 46.151 55.479 1.00 16.94 В 0 ATOM 10273 0 THR 557 53.754 N 46.272 1.00 16.56 В ATOM 10274 N VAL 558 107.348 53.964 1.00 14.93 B C ATOM 10275 CA VAL 558 107.049 47.682 48.302 52.676 1.00 14.99 C ATOM 10276 CB VAL 558 106.483 B 10277 106.033 49.733 52.940 1.00 13.18 C ATOM CG1 VAL В 558 C 48.247 10278 107.544 51.568 1.00 13.02 B ATOM CG2 VAL 558 C 10279 106.058 47.921 55.109 1.00 15.99 В C VAL 558 ATOM 10280 105.060 47.211 55.238 1.00 13.36 В 0 **ATOM** VAL 558 0 106.348 48.923 55.941 1.00 15.43 N **ATOM** 10281 N PHE 559 10282 105.484 49.269 57.069 1.00 14.56 В C ATOM CA PHE 559 106.303 58.173 10283 PHE 49.933 1.00 12.72 В C **ATOM** CB 559 10284 105.469 50.504 59.282 1.00 11.04 В C **ATOM** CG PHE 559 C 10285 CD1 PHE 105.064 49.712 60.347 1.00 10.65 В **ATOM** 559 CD2 PHE 51.833 59.244 1.00 12.10 В C 10286 105.056 ATOM 559 1.00 8.83 CE1 PHE 61.356 C 10287 559 50.232 B ATOM 104.260 Ċ 60.252 1.00 10.43 10288 CE2 PHE 52.360 В **ATOM** 559 104.251

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ATO ATO ATO ATO ATO ATO ATO ATO ATO ATO	DM 10291 DM 10293 DM 10294 DM 10295 DM 10296 DM 10297 DM 10297 DM 10298 DM 10300 DM 10301 DM 10302 DM 10303 DM 10304 DM 10305 DM 10308 DM 10309 DM 10310 DM 10311 DM 10312 DM 10313 DM 10314 DM 10315 DM 10313 DM 10314 DM 10317 DM 10313 DM 10314 DM 10317 DM 10313 DM 10314 DM 10317 DM 10318 DM 10319 DM 10320 DM 10321 DM 10321 DM 10321 DM 10321 DM 10323 DM 10323 DM 10323 DM 10323 DM 103330 DM 10331 DM 103331 DM 1033331 DM 103331 DM 103331 DM 103331 DM 103331 DM 103331 DM 1033331 DM 1033331 DM 1033331 DM 1033331 DM 10333331 DM 10333331 DM 10333331 DM 10333331 DM 10333331 DM 103333331 DM 103333331 DM 10333333333333333333333333333333333333	O N CA CB CG CD1 CD2 C O N CA CB CG CD1 CCD2 C O N CA CB CG CD1 CCD2 C O N CA CB CCD2 CCD1 CCCCCCCCCCCCCCCCCCCCCCCCCCCCC	LEU LEU ASN ASN ASN ASN ASN TRP	559 560 560 560 560 560 560 560 560	104. 395 104. 696 103. 137 102. 029 101. 354 102. 248 101. 491 102. 322 103. 126 103. 203 103. 887 100. 962 100. 661 100. 403 99. 325 99. 626 100. 694 100. 901 100. 275 98. 114 97. 987 97. 222 96. 071 96. 462 96. 924 97. 566 96. 582 94. 818 94. 712 93. 872 92. 616 91. 770 90. 365 89. 623 88. 330 89. 927 89. 512 88. 289 87. 346 88. 951 87. 673 92. 880 92. 279 93. 790 94. 124 95. 216 94. 585 94. 256 95. 332	51. 255 49. 907 50. 744 50. 117 49. 988 49. 421 48. 486 48. 828 50. 090 47. 915 50. 100 52. 183 52. 551 53. 875 53. 875 53. 875 53. 875 53. 875 53. 875 53. 875 53. 875 53. 875 50. 132 49. 309 49. 157 49. 823 49. 309 49. 157 50. 132 49. 719 48. 721 48. 684 47. 856 50. 237 47. 816 46. 980 48. 919 48. 562 48. 161 46. 186 46. 187 48. 037 48. 037	56. 592 56. 865 56. 865 56. 421 55. 185 53. 954 52. 755 51. 999 51. 002 50. 614 50. 421 57. 486 58. 392 59. 100 60. 698 61. 319 57. 475 56. 577 55. 220 57. 465 57. 465 58. 178 58. 191 58. 191 58. 190 58.	1. 00 14. 21 1. 00 14. 64 1. 00 13. 77 1. 00 14. 06 1. 00 12. 20 1. 00 11. 36 1. 00 10. 73 1. 00 13. 38 1. 00 14. 76 1. 00 19. 68 1. 00 16. 46 1. 00 13. 62 1. 00 13. 55 1. 00 11. 68 1. 00 12. 53 1. 00 8. 41 1. 00 10. 22 1. 00 12. 53 1. 00 12. 53 1. 00 13. 62 1. 00 15. 36 1. 00 15. 36 1. 00 14. 07 1. 00 14. 26 1. 00 15. 38 1. 00 14. 89 1. 00 15. 38 1. 00 14. 89 1. 00 15. 38 1. 00 15. 38 1. 00 15. 38 1. 00 15. 38 1. 00 15. 38 1. 00 15. 38 1. 00 15. 38 1. 00 15. 38 1. 00 15. 35 1. 00 15. 35 1. 00 15. 35 1. 00 15. 35 1. 00 15. 35 1. 00 15. 35 1. 00 15. 35 1. 00 15. 35 1. 00 15. 35 1. 00 15. 35 1. 00 15. 35 1. 00 15. 35 1. 00 15. 35 1. 00 15. 58 1. 00 15. 58 1. 00 15. 58 1. 00 17. 65 1. 00 18. 97 1. 00 18. 97 1. 00 18. 97 1. 00 18. 92 1. 00 17. 73	CONCCCNCNCONCCCCCCCONCCCONCONCCCCCONCCCCONCCCCONCCCCONCCCCONCCCCONCCCCONCCCCONCCCCONCCCCONCCCCONCCCCONCCCCONCCCCONCCCCONCCCCONCCCCCONCCCCCONCCCCCONCCCCCONCCCCONCCCCCONCCCCCONCCCCONCCCCCC	
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				FΙ	G. 4 -	2 1 2			(Convinuou)
ATOM	10339	CA 7	THR 56	5 95.81	7 48. 259	60.159	1.00 17.29	В	С
ATOM	10333		THR 56			60. 294	1.00 17.13	В	č
ATOM	10341		THR 56			59. 330	1.00 20.36	B	Ŏ
ATOM	10342	CG2 7				61.676	1.00 18.23	B	Č
ATOM	10343		THR 56			61.157	1.00 15.84	В	С
ATOM	10344		THR 56			62.249	1.00 14.07	В	0
ATOM	10345		TYR 56			60.781	1.00 15.76	В	N
ATOM	10346	CA 1	TYR 56	92.45		61.664	1.00 17.74	В	С
ATOM	10347		ryr 56			61.177	1.00 15.61	В	С
ATOM	10348		TYR 56			61.311	1.00 17.40	В	C
ATOM	10349	CD1 T				60. 195	1.00 17.77	В	C
ATOM	10350	CE1 T				60.310	1.00 15.12	В	C
ATOM	10351	CD2 T				62.556	1.00 18.30	В	C
ATOM	10352	CE2 T				62.682	1.00 17.35	В	C
ATOM	10353		FYR 56			61.550	1.00 17.10	В	C
ATOM	10354		FYR 560 FYR 560			61.662	1.00 17.63	В	0
ATOM ATOM	10355 10356		FYR 560 FYR 560			61. 777 62. 871	1.00 19.12 1.00 20.12	B B	C 0
ATOM	10357		LEU 56'			60. 654	1.00 20.12	В	N N
ATOM	10358		LEU 56'			60. 648	1.00 19.06	В	Č
ATOM	10359		EU 56'			59. 223	1.00 13.00	В	Č
ATOM	10360		EU 56'			58. 284	1.00 18.48	В	Č
ATOM	10361	CD1 L				56. 889	1.00 19.22	В	č
ATOM	10362	CD2 I				58. 835	1.00 15.78	\tilde{B}	č
ATOM	10363		EU 56'			61.544	1.00 20.80	B	Č
ATOM	10364	0 L	LEU 56'			62.157	1.00 23.88	В	0
ATOM	10365		ALA 568			61.628	1.00 19.62	В	N
ATOM	10366		\LA 568			62.466	1.00 20.08	В	C
ATOM	10367		LA 568			61.907	1.00 18.06	В	C
ATOM	10368		LA 568			63.924	1.00 20.52	В	C
ATOM	10369		LA 568			64. 849	1.00 20.37	В	0
ATOM	10370		SER 569			64. 128	1.00 20.79	В	N
ATOM	10371		SER 569			65.474	1.00 21.75	В	C
ATOM	10372		SER 569			65. 401	1.00 21.85	В	C
ATOM ATOM	10373 10374		SER 569 SER 569			66.657	1.00 22.64	В	0 .
ATOM	10374		SER 569 SER 569			66. 267 67. 470	1.00 22.83	В	C
ATOM	10376		HR 570			65.589	1.00 22.38 1.00 22.26	В	0 N
ATOM	10377		HR 570			66. 232	1.00 22.20	B B	N C
ATOM	10378		HR 570			65.797	1.00 21.40	В	C
ATOM	10379	OG1 T				66. 188	1.00 13.31	В	0
ATOM	10380	CG2 T				66. 430	1.00 17.96	В	Č
ATOM	10381		HR 570			65. 974	1.00 24.43	В	č
ATOM	10382		HR 570			66. 894	1.00 27.79	B	ŏ
ATOM	10383		LU 571	89.001		64.727	1.00 23.34	B	Ň
ATOM	10384	CA G	LU 571	88. 030	44. 280	64.415	1.00 21.95	В	Ċ
ATOM	10385		LU 571			62.998	1.00 22.83	В	С
ATOM	10386		LU 571			62. 709	1.00 24.63	В	С
ATOM	10387	CD G	LU 571	85. 957	46.357	63. 696	1.00 25.17	В	С

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				FIG. 4-213	(Continued)
ATOM	10388	OE1 GL	J 571	85. 236 45. 509 64. 258 1. 00 28. 12 B	0
ATOM	10389	OE2 GL	571	85. 834 47. 580 63. 897 1. 00 26. 28 B	0
ATOM	10390	C GL		88.606 42.874 64.554 1.00 21.35 B	С
ATOM	10391	0 GL		87. 903 41. 887 64. 362 1. 00 19. 91 B	0
ATOM	10392	N ASI		89. 887 42. 784 64. 894 1. 00 22. 55 B	N
ATOM	10393	CA ASI		90. 539 41. 491 65. 043 1. 00 21. 58 B	C
ATOM	10394	CB ASI		89. 998 40. 744 66. 255 1. 00 23. 76 B	C
ATOM	10395	CG ASI		90. 523 41. 303 67. 552 1. 00 27. 80 B	C
ATOM	10396	OD1 ASI		90. 053 42. 335 68. 035 1. 00 30. 34 B	0
ATOM	10397	ND2 ASI		91.522 40.634 68.121 1.00 30.31 B	N C
ATOM	10398	C ASI		90.347 40.639 63.806 1.00 21.12 B 90.112 39.436 63.903 1.00 20.16 B	0
ATOM ATOM	10399 10400	O ASI N ILI		90. 445 41. 280 62. 645 1. 00 19. 59 B	N N
ATOM	10400	CA ILI		90.311 40.604 61.365 1.00 18.06 B	C
ATOM	10401	CB ILI		89. 509 41. 456 60. 382 1. 00 18. 14 B	č
ATOM	10403	CG2 ILI		89. 371 40. 735 59. 057 1. 00 18. 53 B	č
ATOM	10404	CG1 ILI		88.143 41.778 60.970 1.00 19.49 B	Č
ATOM	10405	CD1 ILI		87. 336 42. 735 60. 131 1. 00 20. 04 B	Č
ATOM	10406	C ILI		91. 706 40. 425 60. 777 1. 00 18. 47 B	Č
ATOM	10407	0 ILI		92.480 41.376 60.739 1.00 19.08 B	0
ATOM	10408	N ILI	574	92. 038 39. 216 60. 337 1. 00 17. 57 B	N
ATOM	10409	CA ILI		93. 340 38. 978 59. 724 1. 00 18. 02 B	С
ATOM	10410	CB ILI		93. 724 37. 494 59. 740 1. 00 19. 09 B	, C
ATOM	10411	CG2 ILI		94. 950 37. 280 58. 870 1. 00 20. 13 B	C
ATOM	10412	CG1 ILI		94.004 37.031 61.172 1.00 21.02 B	C
ATOM	10413	CD1 ILI		94. 330 35. 553 61. 282 1. 00 20. 47 B	C
ATOM	10414	C ILI		93. 298 39. 423 58. 265 1. 00 17. 84 B	C
ATOM	10415	O ILI		92. 444 38. 981 57. 500 1. 00 19. 48 B	0
ATOM ATOM	10416 10417	N VAI CA VAI		94. 217 40. 296 57. 876 1. 00 17. 13 B 94. 254 40. 777 56. 498 1. 00 16. 42 B	N C
ATOM	10417	CB VAL		94.254 40.777 56.498 1.00 16.42 B 94.354 42.308 56.430 1.00 16.55 B	C C
ATOM	10419	CG1 VAI		94. 271 42. 753 54. 985 1. 00 16. 06 B	Č
ATOM	10420	CG2 VAI		93. 242 42. 948 57. 261 1. 00 15. 54 B	č
ATOM	10421	C VAI		95. 452 40. 187 55. 786 1. 00 16. 02 B	č
ATOM	10422	O VAI		96. 592 40. 488 56. 124 1. 00 16. 68 B	ŏ
ATOM	10423	N ALA		95. 186 39. 344 54. 797 1. 00 16. 21 B	Ň
ATOM	10424	CA ALA		96. 246 38. 683 54. 056 1. 00 15. 22 B	
ATOM	10425	CB ALA		96. 062 37. 176 54. 127 1. 00 12. 38 B	Č
ATOM	10426	C ALA		96. 330 39. 117 52. 601 1. 00 15. 92 B	С
ATOM	10427	0 ALA		95. 397 39. 710 52. 046 1. 00 16. 20 B	0
ATOM	10428	N SEF		97. 470 38. 811 51. 996 1. 00 14. 35 B	N
ATOM	10429	CA SEF		97. 722 39. 123 50. 606 1. 00 13. 57 B	C
ATOM	10430	CB SEF		98. 368 40. 495 50. 474 1. 00 13. 58 B	C
ATOM	10431	OG SEF		97. 456 41. 504 50. 866 1. 00 16. 22 B	0
ATOM	10432	C SEF		98. 642 38. 045 50. 069 1. 00 13. 24 B	C
ATOM	10433	O SEF		99. 497 37. 522 50. 788 1. 00 13. 05 B	0
ATOM	10434	N PHE		98. 462 37. 712 48. 800 1. 00 11. 98 B	N
ATOM ATOM	10435 10436	CA PHE		99. 262 36. 676 48. 183 1. 00 11. 24 B	C
AIUM	10430	CB PHE	910	98. 418 35. 407 48. 079 1. 00 11. 42 B	C

					(Continued)
				FIG. 4-214	
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	10437 10438 10439 10440 10441 10442 10443 10444 10445 10446 10447 10448 10449 10450 10451 10452	CD1 PCD2 PCE1 PCE2 PCZ PCZ PCC PCCA PCCA PCCA PCCA PCCA PC	PHE 578 PHE 578 PHE 578 PHE 578 PHE 578 ASP 578	100. 196 33. 628 48. 152 1. 00 10. 29 B 98. 697 33. 679 46. 280 1. 00 10. 36 B 100. 805 32. 483 47. 640 1. 00 11. 15 B 99. 297 32. 537 45. 762 1. 00 11. 72 B 100. 354 31. 936 46. 446 1. 00 10. 87 B 99. 746 37. 096 46. 805 1. 00 10. 56 B 99. 002 37. 704 46. 039 1. 00 10. 76 B 101. 005 36. 780 46. 516 1. 00 11. 14 B 101. 617 37. 069 45. 227 1. 00 9. 94 B 103. 008 37. 682 45. 401 1. 00 9. 15 B 102. 957 39. 090 45. 954 1. 00 13. 00 B 102. 053 39. 842 45. 532 1. 00 14. 87 B 103. 816 39. 451 46. 796 1. 00 11. 19 B 101. 734 35. 741 44. 488 1. 00 11. 60 B 102. 633 34. 927 44. 753<	C C C C C C C C C C C C C C C C C C C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	10453 10454 10455 10456 10457 10458 10459 10460 10461	CA CO	HY 588 HY 588 HY 588 HY 588 HRG 58 ARG 58 ARG 58 ARG 58 ARG 58	100. 838 34. 274 42. 815 1. 00 11. 96 B 101. 458 34. 470 41. 450 1. 00 13. 34 B 102. 269 35. 376 41. 227 1. 00 12. 96 B 101. 080 33. 611 40. 521 1. 00 14. 18 B 101. 615 33. 714 39. 187 1. 00 15. 34 B 101. 085 32. 570 38. 338 1. 00 13. 67 B 101. 809 31. 283 38. 666 1. 00 15. 30 B 101. 172 30. 076 38. 023 1. 00 14. 62 B	N C C O N C C C C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	10462 10463 10464 10465 10466 10467 10468 10469 10470	CZ A NH1 A NH2 A C A N O CA C		99. 186 28. 672 38. 330 1. 00 13. 69 B 99. 467 28. 024 37. 207 1. 00 13. 99 B 98. 112 28. 348 39. 036 1. 00 12. 41 B 101. 237 35. 069 38. 624 1. 00 17. 21 B 100. 175 35. 615 38. 934 1. 00 17. 96 B 102. 128 35. 628 37. 817 1. 00 18. 14 B 101. 868 36. 933 37. 258 1. 00 17. 73 B 102. 454 37. 998 38. 159 1. 00 16. 81 B	N C N C O N C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	10471 10472 10473 10474 10475 10476 10477 10478 10479 10480 10481 10482 10483	N S CA S CB S C S C C S C C C C C C C C C C C	GLY 58 SER 58 SER 58 SER 58 SER 58 SER 58 GLY 58 GLY 58 GLY 58 GLY 58 GLY 58 TYR 58 TYR 58 TYR 58 TYR 58	102.835 37.625 39.378 1.00 15.90 B 103.423 38.588 40.309 1.00 16.60 B 103.437 38.024 41.730 1.00 17.47 B 104.229 36.856 41.811 1.00 21.54 B 104.841 38.901 39.841 1.00 15.56 B 105.389 38.176 39.013 1.00 17.79 B 105.441 39.970 40.359 1.00 14.64 B 106.776 40.334 39.908 1.00 13.05 B 107.969 40.158 40.831 1.00 12.28 B 107.851 39.648 41.949 1.00 11.78 B 109.129 40.583 40.325 1.00 12.34 B	0 N C C O N C O N C
MOTA MOTA	10484 10485		TYR 58 TYR 58		C C

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					(Continued)
				FIG. 4-215	(Continued)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	10486 10487 10488 10489 10490 10491 10492 10493 10494 10495 10496 10500 10501 10502 10503 10504 10505 10506 10507 10508 10509 10511 10512 10513 10514 10515 10518 10518 10519 10522	CD1 TYR CE1 TYR CE2 TYR CE2 TYR C TYR C TYR C TYR C TYR C TYR C GLN CB GLN CB GLN CB GLN CC GLY CC CC LYS C	585 585 585 585 586 586 586 586 586 586	110. 370 43. 694 41. 297 1. 00 12. 30 B 109. 756 44. 891 40. 979 1. 00 12. 43 B 108. 408 42. 983 42. 478 1. 00 10. 95 B 107. 783 44. 179 42. 167 1. 00 12. 28 B 108. 459 45. 126 41. 418 1. 00 13. 31 B 107. 831 46. 306 41. 109 1. 00 14. 33 B 110. 883 39. 141 41. 394 1. 00 12. 01 B 111. 673 38. 979 42. 319 1. 00 13. 01 B 110. 413 38. 144 40. 655 1. 00 11. 45 B 110. 787 36. 763 40. 906 1. 00 11. 62 B 109. 639 36. 071 41. 641 1. 00 10. 30 B 109. 178 36. 854 42. 867 1. 00 14. 38 B 107. 749 36. 533 43. 295 1. 00 15. 36 B 111. 118 36. 023 39. 602 1. 00 12. 14 B 106. 835 37. 478 43. 060 1. 00 12. 85 B 111.	Continued) C C C C C C C C C C C C C C C C C C
ATOM ATOM	10519 10520	CD LYS CE LYS	589 589	109. 526 28. 579 35. 940 1. 00 32. 47 B 108. 753 27. 273 36. 111 1. 00 33. 79 B	. C
ATOM ATOM ATOM	10521 10522 10523	NZ LYS C LYS O LYS	589 589 589	109. 605 26. 232 36. 771 1. 00 35. 98 B 107. 290 32. 362 35. 536 1. 00 20. 94 B 106. 244 31. 781 35. 242 1. 00 23. 79 B	N C O
ATOM ATOM ATOM	10524 10525 10526	N ILE CA ILE	590 590	107. 384 33. 212 36. 552 1. 00 18. 06 B 106. 237 33. 523 37. 379 1. 00 14. 07 B	N C
ATOM ATOM	10527 10528	CG2 ILE CG1 ILE	590 590 590	106. 681 33. 901 38. 814 1.00 11. 33 B 105. 585 34. 654 39. 538 1.00 9. 61 B 107. 057 32. 635 39. 585 1.00 10. 89 B	C C C
ATOM ATOM ATOM	10529 10530 10531	CD1 ILE C ILE O ILE	590 590 590	107. 750 32. 888 40. 897 1.00 7. 05 B 105. 461 34. 682 36. 753 1. 00 15. 70 B 104. 254 34. 583 36. 511 1. 00 16. 31 B	C C O
ATOM ATOM	10532 10533	N MET CA MET	591 591	106. 159 35. 774 36. 465 1. 00 15. 00 B 105. 506 36. 948 35. 907 1. 00 14. 79 B	N C
ATOM	10534	CB MET	591	106.512 38.088 35.759 1.00 14.22 B	С

				FI	G. 4-	2 1 6			(Continued)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM	10535 10536 10537 10538 10539 10540 10541	SD M CE M C M O M N H	ÆT 591 ÆT 591 ÆT 591 ÆT 591 ÆT 591 HIS 592	107. 027 107. 813 104. 788 103. 643 2 105. 451	40. 830 40. 502 36. 699 37. 113 36. 022	35. 581 35. 526 33. 933 34. 582 34. 418 33. 647 32. 343	1.00 18.55 1.00 17.84 1.00 16.39 1.00 14.86 1.00 14.45 1.00 14.66 1.00 14.33	B B B B B	C S C C O N C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM	10542 10543 10544 10545 10546 10547 10548	CB H CG H CD2 H ND1 H CE1 H NE2 H C H	IIS 592	2 105. 962 2 106. 753 2 106. 626 2 107. 810 2 108. 300 2 107. 598 2 103. 859	35. 424 36. 626 37. 933 36. 555 37. 765 38. 620 34. 569	31. 332 30. 922 31. 252 30. 041 29. 845 30. 567 32. 355	1.00 15.14 1.00 17.56 1.00 17.20 1.00 17.84 1.00 16.59 1.00 16.88 1.00 15.17	B B B B B	C C C N C N C
ATOM ATOM ATOM ATOM ATOM ATOM	10549 10550 10551 10552 10553 10554 10555	N A CA A CB A C A O A N I	IIS 592 LA 593 LA 593 LA 593 LA 593 LA 593 LE 594	103.708 102.775 102.690 101.393 100.647 101.043	33. 917 32. 810 32. 353 33. 195 32. 335 34. 478	31. 344 33. 500 33. 615 35. 060 33. 106 32. 631 33. 207	1.00 15.89 1.00 15.86 1.00 14.02 1.00 13.60 1.00 15.66 1.00 17.83 1.00 16.63	B B B B B	O N C C C O N
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	10556 10557 10558 10559 10560 10561 10562 10563	CB I CG2 I CG1 I CD1 I C I O I	LE 594	99. 035 98. 506 100. 006 100. 533 99. 748 98. 884	35. 017 36. 915 37. 882 35. 689 36. 525	32. 745 33. 791 34. 932 34. 321 33. 274 31. 413 31. 160 30. 558	1. 00 16. 87 1. 00 15. 87 1. 00 16. 36 1. 00 16. 86 1. 00 16. 67 1. 00 17. 96 1. 00 19. 03 1. 00 17. 93	B B B B B B	C C C C C O N
ATOM ATOM ATOM ATOM ATOM ATOM ATOM	10564 10565 10566 10567 10568 10569	CA A CB A CG A OD1 A ND2 A C A	ASN 595 ASN 595 ASN 595 ASN 595	100. 802 102. 140 102. 291 102. 320 102. 377 99. 659	36. 050 35. 737 36. 441 37. 668 35. 667 35. 641	29. 263 28. 592 27. 260 27. 198 26. 184 28. 330	1.00 19.09 1.00 19.22 1.00 19.91 1.00 19.01 1.00 19.95 1.00 19.09 1.00 19.31	B B B B B	C C C O N C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM	10571 10572 10573 10574 10575 10576 10577	N A CA A CB A CG A CD A NE A	RG 596	98. 933 97. 799 98. 212 99. 233 99. 655 98. 553		27. 814 26. 911 25. 677	1. 00 19. 66 1. 00 20. 07 1. 00 17. 78 1. 00 17. 26 1. 00 17. 14 1. 00 17. 97 1. 00 19. 85	B B B B B	N C C C C N C
ATOM ATOM ATOM ATOM ATOM ATOM	10578 10579 10580 10581 10582 10583	NH1 A NH2 A C A O A N A	RG 596	98. 671 97. 060 96. 692 95. 731 96. 811	37. 005 35. 486 35. 655 35. 213 35. 529 34. 770	21. 640 21. 045 27. 632 27. 005 28. 948 29. 714	1.00 21.47 1.00 18.12 1.00 21.03 1.00 22.67 1.00 20.90 1.00 20.85	B B B B B	N N C O N C

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				FIG. 4-218	(Continued)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	10633 10634 10635 10636 10637 10638 10639 10640 10641 10642	CA VAL CB VAL CG1 VAL CG2 VAL C VAL O VAL N GLU CA GLU CB GLU CG GLU	603 603 603 603 603 604 604 604	92. 696 34. 413 39. 984 1. 00 21. 62 B 91. 513 34. 471 38. 999 1. 00 21. 51 B 90. 233 34. 055 39. 701 1. 00 19. 24 B 91. 380 35. 876 38. 442 1. 00 21. 00 B 92. 643 33. 073 40. 716 1. 00 22. 35 B 92. 160 32. 989 41. 848 1. 00 21. 06 B 93. 141 32. 031 40. 059 1. 00 22. 98 B 93. 182 30. 702 40. 656 1. 00 26. 04 B 93. 721 29. 681 39. 645 1. 00 28. 46 B 92. 956 29. 671 38. 326 1. 00 35. 94 B	C C C C O N C C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	10643 10644 10645 10646 10647 10648 10649 10650 10651	CD GLU OE1 GLU OE2 GLU O GLU O GLU N ASP CA ASP CB ASP CG ASP	604 604 604 604 605 605 605	93. 559 28. 742 37. 273 1. 00 40. 17 B 93. 215 28. 911 36. 076 1. 00 40. 47 B 94. 360 27. 844 37. 637 1. 00 41. 61 B 94. 072 30. 705 41. 905 1. 00 24. 63 B 93. 657 30. 255 42. 976 1. 00 25. 47 B 95. 286 31. 234 41. 775 1. 00 22. 17 B 96. 213 31. 255 42. 900 1. 00 21. 12 B 97. 568 31. 827 42. 463 1. 00 23. 09 B 98. 263 30. 958 41. 414 1. 00 24. 43 B	C 0 0 C 0 N C C C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	10652 10653 10654 10655 10656 10657 10658 10659 10660	OD1 ASP OD2 ASP C ASP O ASP N GLN CA GLN CB GLN CG GLN CD GLN	605 605 605 606 606 606 606	97. 894 29. 774 41. 266 1. 00 26. 59 B 99. 188 31. 453 40. 742 1. 00 25. 60 B 95. 712 31. 967 44. 159 1. 00 19. 42 B 96. 099 31. 598 45. 260 1. 00 19. 67 B 94. 868 32. 983 44. 014 1. 00 17. 23 B 94. 337 33. 673 45. 192 1. 00 16. 41 B 93. 576 34. 951 44. 795 1. 00 17. 09 B 94. 407 36. 070 44. 165 1. 00 15. 81 B 95. 332 36. 748 45. 162 1. 00 15. 36 B	0 0 C 0 N C C C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	10661 10662 10663 10664 10665 10666 10667 10668	OEI GLN NE2 GLN C GLN O GLN N ILE CA ILE CB ILE CG2 ILE CG1 ILE	606 606 606 606 607 607 607 607	94. 879 37. 283 46. 173 1. 00 13. 19 B 96. 637 36. 730 44. 878 1. 00 14. 39 B 93. 360 32. 706 45. 878 1. 00 15. 71 B 93. 337 32. 583 47. 102 1. 00 14. 30 B 92. 549 32. 030 45. 070 1. 00 13. 95 B 91. 584 31. 076 45. 583 1. 00 13. 95 B 90. 772 30. 437 44. 448 1. 00 12. 90 B 89. 925 29. 294 44. 996 1. 00 11. 78 B 89. 909 31. 504 43. 773 1. 00 12. 90 B	O N C O N C C C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	10669 10670 10671 10672 10673 10674 10675 10676 10677 10678	CD1 ILE C ILE O ILE N GLU CA GLU CB GLU CG GLU CD GLU OE1 GLU	607 607 607 608 608 608 608 608	89. 162 31. 016 42. 560 1. 00 11. 00 B 92. 330 29. 985 46. 318 1. 00 15. 04 B 92. 008 29. 670 47. 462 1. 00 15. 40 B 93. 331 29. 413 45. 652 1. 00 16. 29 B 94. 144 28. 359 46. 246 1. 00 18. 48 B 95. 180 27. 864 45. 235 1. 00 18. 74 B 96. 164 26. 851 45. 792 1. 00 22. 43 B 95. 498 25. 557 46. 213 1. 00 29. 00 B 96. 096 24. 817 47. 032 1. 00 32. 52 B	C C O N C C C C
ATOM ATOM ATOM	10679 10680 10681	OE2 GLU C GLU O GLU	608 608 608	94. 382 25. 274 45. 721 1. 00 31. 62 B 94. 848 28. 889 47. 501 1. 00 20. 58 B 95. 114 28. 138 48. 446 1. 00 23. 01 B	0 C 0

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			(Continued)
		FIG. 4 - 219	
ATOM 10687 ATOM 10688 ATOM 10689 ATOM 10690 ATOM 10691 ATOM 10692 ATOM 10693 ATOM 10694 ATOM 10695 ATOM 10696 ATOM 10697 ATOM 10698 ATOM 10699	N ALA 609 CA ALA 609 CB ALA 609 C ALA 609 O ALA 609 N ALA 610 CA ALA 610 CB ALA 610 C ALA 610 N ARG 611 CA ARG 611 CB ARG 611 CB ARG 611 CC ARG 611 NE ARG 611 NE ARG 611 NE ARG 611 NE ARG 611 NH ARG 611	F I G. 4 - 2 1 9 95. 150 30. 183 47. 506 1. 00 19. 99 95. 811 30. 789 48. 646 1. 00 21. 28 96. 269 32. 196 48. 310 1. 00 19. 81 94. 826 30. 819 49. 797 1. 00 21. 63 95. 152 30. 426 50. 915 1. 00 21. 88 93. 618 31. 286 49. 516 1. 00 23. 07 92. 580 31. 358 50. 535 1. 00 25. 56 91. 317 31. 963 49. 957 1. 00 25. 38 92. 300 29. 952 51. 024 1. 00 26. 13 92. 256 29. 694 52. 223 1. 00 25. 97 92. 119 29. 044 50. 073 1. 00 28. 12 91. 838 27. 647 50. 374 1. 00 28. 88 91. 886 26. 826 49. 087 1. 00 27. 27 91. 518 25. 372 49. 260 1. 00 28. 40 91. 547 24. 668 47. 925 1. 00 30. 54 90. 501 25. 152 47. 028 1. 00 33. 73 90. 628 25. 223 45. 706 1. 00 38. 00	B N B C B C B C B C B C B C B C B C B C B C
ATOM 10700 ATOM 10701 ATOM 10702 ATOM 10703 ATOM 10704 ATOM 10705	NH2 ARG 611 C ARG 611 O ARG 611 N GLN 612 CA GLN 612 CB GLN 612 CG GLN 612	89. 615 25. 645 44. 956 1. 00 37. 15 92. 826 27. 082 51. 391 1. 00 29. 24 92. 446 26. 330 52. 287 1. 00 30. 51 94. 092 27. 452 51. 260 1. 00 30. 24 95. 105 26. 965 52. 182 1. 00 30. 75 96. 491 27. 029 51. 532 1. 00 29. 62 96. 738 25. 866 50. 581 1. 00 31. 27	B N B C B O B N B C B C B C B C
ATOM 10707 ATOM 10708 ATOM 10709 ATOM 10710 ATOM 10711 ATOM 10712	CD GLN 612 OE1 GLN 612 NE2 GLN 612 C GLN 612 O GLN 612 N PHE 613 CA PHE 613	98. 183 25. 741 50. 150 1. 00 32. 19 99. 097 25. 778 50. 979 1. 00 32. 20 98. 400 25. 578 48. 848 1. 00 31. 86 95. 109 27. 691 53. 524 1. 00 31. 36 95. 441 27. 095 54. 545 1. 00 32. 39 94. 740 28. 969 53. 533 1. 00 31. 39 94. 705 29. 717 54. 784 1. 00 30. 50	B C B O B N B C B O B N
ATOM 10714 ATOM 10715 ATOM 10716 ATOM 10717 ATOM 10718 ATOM 10719 ATOM 10720	CB PHE 613 CG PHE 613 CD1 PHE 613 CD2 PHE 613 CE1 PHE 613 CE2 PHE 613 CZ PHE 613	94. 527 31. 217 54. 538 1. 00 30. 43 95. 651 31. 853 53. 775 1. 00 31. 06 96. 974 31. 532 54. 058 1. 00 32. 48 95. 385 32. 805 52. 796 1. 00 30. 25 98. 024 32. 156 53. 371 1. 00 32. 97 96. 419 33. 432 52. 109 1. 00 31. 17 97. 742 33. 109 52. 394 1. 00 32. 13	B C B C B C B C B C B C B C B C
ATOM 10722 (ATOM 10723 II ATOM 10724 ATOM 10725 (ATOM 10726 (ATOM 10727 (ATOM 10728 (ATOM 10729 II ATOM 10729 II A	C PHE 613 O PHE 613 N SER 614 CA SER 614 CB SER 614 OG SER 614 C SER 614 O SER 614 N LYS 615 CA LYS 615	93. 531 29. 214 55. 607 1. 00 30. 36 93. 572 29. 216 56. 830 1. 00 28. 96 92. 478 28. 786 54. 923 1. 00 31. 88 91. 292 28. 286 55. 600 1. 00 34. 43 90. 141 28. 104 54. 607 1. 00 34. 30 90. 419 27. 055 53. 697 1. 00 34. 39 91. 609 26. 953 56. 264 1. 00 35. 74 90. 908 26. 519 57. 178 1. 00 37. 21 92. 670 26. 307 55. 797 1. 00 36. 52 93. 079 25. 030 56. 350 1. 00 37. 25	B C B O B C B O B C B O B C B O B C B O B C B O C B O C C C C

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						(Continued)
					FIG. 4-222	
ATOM ATOM ATOM ATOM ATOM	10829 10830 10831 10832 10833	CD2 CE2 CE3 CD1 NE1	TRP TRP TRP	627 627 627 627 627	89. 641 46. 084 49. 646 1. 00 11. 41 B 90. 725 46. 410 50. 500 1. 00 10. 99 B 89. 121 47. 074 48. 806 1. 00 9. 75 B 90. 198 44. 267 50. 826 1. 00 14. 55 B 91. 046 45. 283 51. 208 1. 00 10. 25 B	C N
ATOM ATOM	10834 10835	CZ2 CZ3	TRP	627 627	91. 289 47. 681 50. 536 1. 00 9. 06 B 89. 685 48. 340 48. 844 1. 00 9. 47 B	C C
MOTA MOTA	10836 10837	CH2 C	TRP	627 627	90. 755 48. 632 49. 702 1. 00 8. 43 B 89. 881 43. 489 47. 433 1. 00 17. 27 B	C
ATOM ATOM	10838	0 · N	TRP GLY	627 628	91. 027 43. 146 47. 732 1. 00 16. 96 B 89. 613 44. 351 46. 459 1. 00 16. 52 B 90. 672 44. 947 45. 675 1. 00 16. 52 B	N
ATOM ATOM ATOM	10840 10841 10842	CA C O	GLY GLY GLY	628 628 628	90. 186 46. 198 44. 975 1. 00 17. 44 B 88. 977 46. 441 44. 887 1. 00 17. 88 B	C
ATOM ATOM	10843 10844	N CA	TRP TRP	629 629	91. 132 46. 989 44. 479 1. 00 15. 93 B 90. 841 48. 235 43. 781 1. 00 15. 93 B	N
ATOM ATOM	10845 10846	CB CG	TRP TRP	629 629	91. 480 49. 395 44. 552 1. 00 13. 57 B 90. 867 50. 763 44. 341 1. 00 14. 96 B	C
ATOM ATOM	10847 10848	CE2	TRP	629 629	90. 389 51. 656 45. 360 1. 00 13. 15 B 89. 944 52. 830 44. 712 1. 00 13. 17 B	C
ATOM ATOM	10849 10850	CE3 CD1	TRP	629 629	90. 296 51. 577 46. 758 1. 00 14. 07 B 90. 694 51. 419 43. 149 1. 00 14. 45 B 90. 141 52. 657 43. 366 1. 00 12. 77 B	С
MOTA MOTA MOTA	10851 10852 10853	NE1 CZ2 CZ3	TRP	629 629 629	89. 411 53. 921 45. 414 1. 00 13. 59 B	C
ATOM ATOM	10854 10855		TRP TRP	629 629	89. 330 53. 820 46. 782 1. 00 15. 16 B 91. 481 48. 074 42. 399 1. 00 17. 34 B	C C
ATOM ATOM	10856 10857	O N	TRP SER	629 630	92. 571 47. 517 42. 285 1. 00 18. 55 B 90. 802 48. 538 41. 354 1. 00 17. 70 B	N
ATOM ATOM	10858 10859	CA CB	SER SER	630 630	91. 309 48. 430 39. 982 1. 00 17. 70 B 92. 649 49. 144 39. 846 1. 00 18. 19 B 92. 574 50. 437 40. 404 1. 00 24. 67 B	C
ATOM ATOM ATOM	10860 10861 10862	0G C 0	SER SER SER	630 630 630	92. 574 50. 437 40. 404 1. 00 24. 67 B 91. 477 46. 977 39. 563 1. 00 17. 40 B 90. 501 46. 235 39. 469 1. 00 18. 69 B	C
ATOM ATOM	10863 10864	N CA	TYR TYR	631 631	92. 712 46. 565 39. 304 1. 00 16. 34 B 92. 951 45. 192 38. 904 1. 00 15. 96 B	N
ATOM ATOM	10865 10866	CB CG	TYR TYR	631 631	94.430 44.973 38.579 1.00 15.36 B 94.689 43.709 37.779 1.00 15.93 B	C
ATOM ATOM	10867 10868	CE1	TYR TYR	631 631	94. 626 42. 450 38. 380 1. 00 15. 38 B 94. 830 41. 287 37. 634 1. 00 16. 25 B	C
ATOM ATOM ATOM	10869 10870 10871		TYR TYR TYR	631 631 631	94. 961 43. 773 36. 409 1. 00 15. 67 B 95. 160 42. 620 35. 655 1. 00 13. 59 B 95. 092 41. 384 36. 270 1. 00 15. 96 B	C
ATOM ATOM	10872 10873	OH C	TYR TYR	631 631	95. 264 40. 243 35. 525 1. 00 14. 59 92. 499 44. 286 40. 049 1. 00 15. 68	0
ATOM ATOM	10874 10875	0 N	TYR GLY	631 632	91. 949 43. 213 39. 824 1. 00 16. 42 B 92. 723 44. 729 41. 281 1. 00 15. 56 B	O N
ATOM ATOM	10876 10877	CA C	GLY GLY	632 632	92. 292 43. 950 42. 429 1. 00 14. 43 B 90. 777 43. 807 42. 398 1. 00 13. 07 B	

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						(Continued)
					FIG. 4-223	(00110111404)
	10050		OY 11	000	00 000 49 771 49 777 1 00 19 0	10 P O
ATOM	10878	0 N	GLY GLY	632 633	90. 239 42. 771 42. 777 1. 00 12. 0 90. 087 44. 855 41. 946 1. 00 12. 5	
ATOM ATOM	10879 10880	N CA	GLY	633	88.637 44.800 41.846 1.00 10.8	
ATOM	10881	C	GLY	633	88. 271 43. 743 40. 818 1. 00 10. 7	
ATOM	10882	ŏ	GLY	633	87. 337 42. 956 40. 986 1. 00 9. 2	
ATOM	10883	Ň	TYR	634	89. 031 43. 729 39. 734 1. 00 11. 3	33 B N
ATOM	10884	CA	TYR	634	88. 822 42. 755 38. 682 1. 00 11. 0	
ATOM	10885	CB	TYR	634	89. 860 42. 951 37. 595 1. 00 7. 3	
ATOM	10886	CG	TYR	634	89. 815 41. 899 36. 526 1. 00 8. 0	04 B C
ATOM	10887		TYR	634	90. 949 41. 162 36. 204 1. 00 7. 5	
ATOM	10888		TYR	634	90. 924 40. 218 35. 189 1. 00 7. 5	
ATOM	10889 10890		TYR TYR	634 634	88. 649 41. 660 35. 805 1. 00 8. 8 88. 615 40. 715 34. 788 1. 00 7. 8	
ATOM ATOM	10891	CZ	TYR	634	89. 756 39. 996 34. 488 1. 00 6. 9	
ATOM	10892	OH	TYR	634	89. 722 39. 039 33. 504 1. 00 8. 0	
ATOM	10893	C	TYR	634	88. 967 41. 358 39. 278 1. 00 13. 0	
ATOM	10894	Ŏ	TYR	634	88. 038 40. 548 39. 222 1. 00 13. 1	
ATOM	10895	N	VAL	635	90.140 41.091 39.858 1.00 14.3	
ATOM	10896	CA	VAL	635	90. 426 39. 796 40. 467 1. 00 13. 3	
ATOM	10897	CB	VAL	635	91. 839 39. 747 41. 093 1. 00 13. 2	
ATOM	10898		VAL	635	91. 995 38. 467 41. 923 1. 00 13. 0	
ATOM	10899		VAL	635	92. 894 39. 782 39. 999 1. 00 8. 0	
ATOM ATOM	10900 10901	C 0	VAL VAL	635 635	89. 412 39. 443 41. 533 1. 00 13. 3 88. 932 38. 320 41. 563 1. 00 15. 0	
ATOM	10901	N	THR	636	89. 091 40. 394 42. 405 1. 00 13. 4	
ATOM	10903	CA	THR	636	88. 108 40. 160 43. 457 1. 00 13. 7	
ATOM	10904	CB	THR	636	87. 788 41. 451 44. 260 1. 00 15. 1	
ATOM	10905	0G1	THR	636	88. 950 41. 886 44. 978 1. 00 15. 2	
ATOM	10906	CG2		636	86.655 41.188 45.259 1.00 13.5	
ATOM	10907	C	THR	636	86. 792 39. 665 42. 862 1. 00 14. 5	
ATOM	10908	0	THR	636	86. 160 38. 750 43. 395 1. 00 15. 2	
ATOM	10909	N	SER	637	86. 373 40. 281 41. 762 1. 00 15. 5	
ATOM	10910	CA	SER	637	85. 120 39. 905 41. 112 1. 00 15. 9	
ATOM ATOM	10911 10912	CB OG	SER SER	637 637	84. 698 40. 974 40. 102 1. 00 16. 8 84. 303 42. 158 40. 766 1. 00 18. 0	
ATOM	10912	C	SER	637	85. 195 38. 558 40. 420 1. 00 16. 5	
ATOM	10914	ŏ	SER	637	84. 250 37. 773 40. 487 1. 00 17. 8	
ATOM	10915	Ň	MET	638	86.309 38.300 39.740 1.00 15.6	
ATOM	10916	CA	MET	638	86.493 37.030 39.052 1.00 15.5	55 B C
ATOM	10917	CB	MET	638	87. 807 37. 033 38. 272 1. 00 15. 9	97 B C
ATOM	10918	CG	MET	638	87. 822 37. 959 37. 067 1. 00 17. 3	88 B C
ATOM	10919	SD	MET	638	86. 715 37. 422 35. 736 1. 00 19. 1	
ATOM	10920	CE	MET	638	87. 806 36. 324 34. 798 1. 00 15. 2	28 B C
ATOM	10921	C	MET	638	86. 511 35. 913 40. 093 1. 00 17. 5	
ATOM	10922 10923	и 0	MET VAL	638	86. 018 34. 807 39. 843 1. 00 17. 4 87. 086 36. 199 41. 260 1. 00 16. 5	
ATOM ATOM	10923	N CA	VAL	639 639	87. 086 36. 199 41. 260 1. 00 16. 5 87. 133 35. 207 42. 317 1. 00 17. 2	
ATOM	10924	CB	VAL	639	88.047 35.640 43.480 1.00 16.7	
ATOM	10926		VAL	639	87. 648 34. 884 44. 757 1. 00 16. 2	
			· - -			-

		٠			(Continued)
				FIG. 4-224	(00111111111111111111111111111111111111
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	10927 10928 10929 10930 10931 10932 10933 10934 10935 10936 10941 10942 10943 10944 10945 10946 10947 10948 10949 10950 10951	CG2 VAL C VAL O VAL N LEU CA LEU CB LEU CG LEU CD1 LEU C LEU O LEU N GLY CA GLY O GLY N SER CA SER CB SER OG SER C SER O SER O SER N GLY C GLY O GLY	639 639 640 640 640 640 641 641 641 642 642 642 643 643	89. 495 35. 335 43. 139 1. 00 14. 45 B 85. 742 34. 919 42. 875 1. 00 17. 57 B 85. 387 33. 760 43. 081 1. 00 18. 52 B 84. 957 35. 964 43. 124 1. 00 16. 90 B 83. 618 35. 766 43. 661 1. 00 17. 42 B 82. 978 37. 098 44. 032 1. 00 17. 45 B 83. 512 37. 699 45. 327 1. 00 17. 52 B 82. 743 38. 962 45. 654 1. 00 14. 30 B 83. 378 36. 677 46. 447 1. 00 15. 97 B 82. 713 35. 020 42. 699 1. 00 17. 81 B 81. 821 34. 284 43. 119 1. 00 20. 73 B 82. 952 35. 198 41. 409 1. 00 18. 14 B 82. 135 34. 526 40. 418 1. 00 17. 51 B 82. 758 33. 235 39. 936 1. 00 17. 52 B 82. 346 32. 697 38. 911 1. 00 15. 15 B 83. 691 <	C C C C C C C C C C C C C C C C C C C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	10952 10953 10954 10955 10956 10957 10958 10959 10960 10961 10962 10963 10964 10965 10966 10967 10968 10969 10970 10971 10972 10973 10975	N SER CA SER CB SER OG SER C SER O SER N GLY CA GLY C GLY O GLY N VAL CB VAL CG1 VAL CG2 VAL C VAL C VAL C VAL C VAL C VAL C C VAL C	644 644 644 644 645 645 645 646 646 647 647 647 647	83. 859 28. 849 43. 772 1. 00 22. 41 B 84. 684 28. 024 44. 656 1. 00 21. 56 B 86. 065 28. 657 44. 833 1. 00 21. 02 B 85. 992 29. 798 45. 666 1. 00 22. 35 B 84. 084 27. 773 46. 037 1. 00 21. 06 B 84. 451 26. 807 46. 707 1. 00 23. 51 B 83. 175 28. 643 46. 469 1. 00 19. 50 B 82. 561 28. 485 47. 774 1. 00 16. 85 B 83. 484 28. 868 48. 920 1. 00 18. 76 B 83. 111 28. 771 50. 090 1. 00 18. 32 B 84. 691 29. 320 48. 591 1. 00 18. 97 B 85. 669 29. 695 49. 612 1. 00 18. 18 B 87. 095 29. 718 49. 029 1. 00 19. 50 B 88. 082 30. 202 50. 086 1. 00 17. 45 B 87. 471 28. 341 48. 516 1. 00 17. 29 B 85. 433 31. 051 50. 266 1. 00 17. 29 B 85. 433 31. 051 50. 266 1. 00 18. 24 B 85. 860 31. 270 51. 396 1. 00 20. 76 B 84. 763 31. 957 49. 561 1. 00 16. 76 B 85. 066 34. 337 49. 094 1. 00 16. 60 B 85. 066 34. 337 49. 094 1. 00 16. 60 B 87. 455 34. 941 49. 553 1. 00 14. 72 B 88. 826 34. 800 49. 317 1. 00 16. 66 B	NCCOCONCCCCCONCCCCCC

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						(Continued)
					FIG. 4-225	
ATOM	10976		PHE	647	88.356 33.170 47.600 1.00 16.73 B	С
ATOM	10977	CZ	PHE	647	89. 278 33. 913 48. 338 1. 00 13. 35 B	C
ATOM	10978	C	PHE	647	83. 068 33. 604 50. 365 1. 00 16. 77 B	C
ATOM	10979	0 N	PHE	647	82. 194 33. 328 49. 551 1. 00 17. 32 B 82. 819 34. 214 51. 515 1. 00 16. 74 B	0 N
ATOM ATOM	10980 10981	N CA	LYS LYS	648 648	82.819 34.214 51.515 1.00 16.74 B 81.466 34.565 51.905 1.00 19.64 B	N C
ATOM	10982	CB	LYS	648	81. 369 34. 634 53. 429 1. 00 19. 84 B	č
ATOM	10983	CG	LYS	648	80.069 35.233 53.911 1.00 21.93 B	č
ATOM	10984	CD	LYS	648	79. 876 35. 060 55. 393 1. 00 23. 19 B	Č .
ATOM	10985	CE	LYS	648	78. 548 35. 645 55. 814 1. 00 24. 97 B	C
ATOM	10986	NZ	LYS	648	78. 180 35. 150 57. 165 1. 00 31. 55 B	N
ATOM	10987	C	LYS	648	81.019 35.900 51.308 1.00 21.05 B	C
ATOM	10988	0	LYS	648	79. 851 36. 070 50. 930 1. 00 20. 25 B	0
ATOM	10989	N	CYS	649	81. 954 36. 842 51. 237 1. 00 20. 69 B	N
ATOM ATOM	10990 10991	CA C	CYS CYS	649 649	81. 670 38. 163 50. 711 1. 00 21. 97 B 82. 928 38. 811 50. 134 1. 00 22. 72 B	C C
ATOM	10991	Ô	CYS	649	84. 054 38. 437 50. 477 1. 00 23. 68 B	0
ATOM	10993	CB	CYS	649	81.124 39.045 51.822 1.00 23.52 B	Č
ATOM	10994	SG	CYS	649	82. 287 39. 215 53. 208 1. 00 26. 89 B	Š
ATOM	10995	N	GLY	650	82. 728 39. 796 49. 267 1. 00 20. 11 B	N
ATOM	10996	CA	GLY	650	83. 850 40. 476 48. 668 1. 00 18. 42 B	С
ATOM	10997	C	GLY	650	83. 484 41. 895 48. 308 1. 00 18. 08 B	C
ATOM	10998	0	GLY	650	82. 308 42. 198 48. 135 1. 00 18. 19 B	0
ATOM	10999	N	ILE	651	84. 490 42. 764 48. 209 1. 00 17. 42 B	N
ATOM ATOM	11000 11001	CA CB	ILE ILE	651 651	84. 284 44. 162 47. 851 1. 00 15. 98 B 84. 632 45. 117 49. 014 1. 00 15. 40 B	C C
ATOM	11001		ILE	651	84. 632 45. 117 49. 014 1. 00 15. 40 B 84. 386 46. 559 48. 589 1. 00 15. 87 B	C
ATOM	11002		ILE	651	83. 789 44. 786 50. 242 1. 00 15. 95 B	Č
ATOM	11004		ILE	651	84. 017 45. 721 51. 411 1. 00 14. 84 B	č
ATOM	11005	C	ILE	651	85. 190 44. 512 46. 679 1. 00 16. 40 B	Č
ATOM	11006	0	ILE	651	86. 404 44. 330 46. 754 1. 00 16. 63 B	0 .
ATOM	11007	N	ALA	652	84. 594 45. 025 45. 608 1. 00 16. 04 B	N
ATOM	11008	CA	ALA	652	85. 330 45. 409 44. 413 1. 00 15. 10 B	C
ATOM	11009	CB	ALA	652	84. 809 44. 629 43. 214 1. 00 16. 38 B	C
ATOM ATOM	11010 11011	C 0	ALA ALA	652 652	85. 190° 46. 908 44. 153 1. 00 15. 88 B 84. 089 47. 399 43. 895 1. 00 14. 37 B	C
ATOM	11011	N	VAL	653	84. 089 47. 399 43. 895 1. 00 14. 37 B 86. 308 47. 630 44. 214 1. 00 15. 73 B	0 N
ATOM	11013	CA	VAL	653	86. 298 49. 070 43. 978 1. 00 15. 50 B	C
ATOM	11014	CB	VAL	653	87. 110 49. 831 45. 055 1. 00 17. 97 B	č
ATOM	11015		VAL	653	87. 050 51. 327 44. 787 1. 00 18. 06 B	č
ATOM	11016	CG2	VAL	653	86. 566 49. 525 46. 446 1. 00 18. 80 B	Č
ATOM	11017	C	VAL	653	86. 905 49. 398 42. 624 1. 00 15. 11 B	C
ATOM	11018	0	VAL	653	88. 071 49. 087 42. 373 1. 00 14. 41 B	0
ATOM	11019	N	ALA	654	86. 106 50. 031 41. 766 1. 00 14. 05 B	N
ATOM	11020	CA	ALA	654	86. 532 50. 438 40. 427 1. 00 12. 10 B	C
ATOM	11021 11022	CB	ALA at a	654 654	87. 424 51. 655 40. 518 1. 00 12. 15 B	C
ATOM ATOM	11022	C 0	ALA ALA	654 654	87. 258 49. 318 39. 700 1. 00 12. 48 B 88. 364 49. 500 39. 192 1. 00 13. 17 B	C
ATOM	11023	N	PRO	655	88. 364 49. 500 39. 192 1. 00 13. 17 B 86. 633 48. 141 39. 626 1. 00 11. 84 B	O N
VIÂN	11007	11	1 110	000	00.000 40.141 03.020 1.00 11.04 D	14

									(Continued)
				FIG	. 4 -	2 2 6			Conumaca
ATOM	11025	CD P	RO 655	85. 273	47. 797	40. 088	1.00 11.50	В	С
ATOM ATOM	11025		RO 655	87. 247	47.003	38. 954	1.00 11.05	B	č
ATOM	11027		RO 655	86.399	45. 841	39. 436	1.00 11.09	B	Č
ATOM	11028		RO 655	85.030	46. 451	39. 428	1.00 8.50	B	Ċ
ATOM	11029		RO 655	87.190	47.102	37.447	1.00 10.92	В	C
ATOM	11030		RO 655	86.383	47.847	36.896	1.00 11.41	В	0
ATOM	11031		AL 656	88.066	46.352	36. 791	1.00 9.60	В	N
ATOM	11032	CA V	AL 656	88.052	46.250	35. 345	1.00 9.08	В	C
ATOM	11033		AL 656	89. 452	45. 888	34. 790	1.00 7.45	В	C C
ATOM	11034	CG1 V		89. 336	45. 163	33. 451	1.00 5.90	В	
ATOM	11035	CG2 V		90. 249	47.146	34. 601	1.00 7.63	В	Č ,
ATOM	11036		AL 656	87.107	45.056	35. 224	1.00 10.20	В	C
ATOM	11037		AL 656	87. 157	44. 152	36. 058	1.00 10.59	В	0
ATOM	11038		ER 657	86. 231	45.038	34. 230	1.00 11.76	В	N C
ATOM	11039		ER 657	85. 313 83. 867	43. 908 44. 375	34. 115 34. 271	1.00 14.03 1.00 13.85	B B	C C
ATOM ATOM	11040 11041		ER 657 ER 657	83. 495	45. 242	33. 218	1.00 15.05	В	0
ATOM	11041		ER 657	85. 456	43. 153	32. 812	1.00 13.07	В	Č
ATOM	11042		ER 657	85. 191	41. 952	32. 743	1.00 17.18	B	ŏ
ATOM	11044		RG 658	85. 887	43. 860	31. 781	1.00 14.15	B	Ň
ATOM	11045		RG 658	86.050	43. 277	30. 459	1.00 13.24	B	Ċ
ATOM	11046		RG 658	84. 768	43. 532	29.670	1.00 14.22	B	Č
ATOM	11047		RG 658	84.763	43.086	28. 231	1.00 18.57	В	C
ATOM	11048		RG 658	83.436	43.470	27.588	1.00 19.40	В	C
ATOM	11049		RG 658	83. 475	43. 338	26. 138	1.00 23.11	В	N ·
ATOM	11050	CZ A	RG 658	82.868	42.376	25. 454	1.00 22.54	В	C
ATOM	11051	NH1 A		82. 167	41.445	26.088	1.00 21.95	В	N
ATOM	11052	NH2 A		82. 955	42.361	24. 131	1.00 22.77	В	N
ATOM	11053		RG 658	87. 242	44.014	29.857	1.00 12.76	В	C
ATOM	11054		RG 658	87. 218	45. 239	29. 733	1.00 11.97	В	0
ATOM	11055		RP 659	88. 282	43. 283	29.476	1.00 11.05	В	N
ATOM	11056		RP 659	89.468	43.942	28. 955	1.00 12.23	В	C
ATOM	11057		RP 659 RP 659	90. 578	42. 918 42. 392	28. 777 30. 112	1.00 11.99 1.00 13.26	B B	C
ATOM ATOM	11058 11059	CD2 T		91. 026 91. 729	43. 120	31. 122	1.00 13.20	В	C C
ATOM	11060	CE2 T		91. 848	42. 271	32. 242	1.00 12.01	В	Č
ATOM	11061	CE3 T		92. 268	44. 412	31. 193	1.00 14.19	В	č
ATOM	11062		RP 659	90. 759	41. 163	30. 644	1.00 13.17	В	č
ATOM	11063	NE1 T		91. 247	41.083	31.920	1.00 13.29	В	Ň
ATOM	11064	CZ2 T		92.489	42.670	33. 424	1.00 13.99	B	Ĉ
ATOM	11065	CZ3 T		92. 909	44.810	32. 373	1.00 13.35	B	č
ATOM	11066	CH2 T		93.011	43.940	33.468	1.00 11.92	В	Č
ATOM	11067	C T	RP 659	89. 338	44.840	27. 730	1.00 13.23	В	Ċ
ATOM	11068		RP 659	90.118	45.766	27. 569	1.00 15.39	В	0
ATOM	11069		LU 660	88. 361	44. 595	26.871	1.00 14.59	В	N
ATOM	11070		LU 660	88. 181	45. 453	25. 708	1.00 15.33	В	Č
ATOM	11071		LU 660	87. 147	44.854	24. 743	1.00 18.10	В	C
ATOM	11072		LU 660	87. 572	43. 527	24. 130	1.00 21.82	В	C
ATOM	11073	CD G	LU 660	86. 452	42.829	23. 386	1.00 25.49	В	С

					(Continued)
		FIC	G. 4 - 22	7	(2) = = = = = = = = = = = = = = = = = =
ATOM 11074 ATOM 11075 ATOM 11077 ATOM 11077 ATOM 11079 ATOM 11080 ATOM 11081 ATOM 11082 ATOM 11083 ATOM 11084 ATOM 11085 ATOM 11086 ATOM 11087 ATOM 11089 ATOM 11090 ATOM 11091 ATOM 11092 ATOM 11093 ATOM 11094 ATOM 11095 ATOM 11095 ATOM 11096 ATOM 11097 ATOM 11097 ATOM 11098 ATOM 11098 ATOM 11098 ATOM 11097 ATOM 11097 ATOM 11098 ATOM 11100 ATOM 11101 ATOM 11102 ATOM 11103 ATOM 11104 ATOM 11106 ATOM 11106 ATOM 11107 ATOM 11108 ATOM 11108	OE2 GLU C GLU C GLU O GL	F I 6 660 86. 087 660 87. 719 660 87. 661 661 87. 371 661 86. 941 661 85. 988 661 84. 599 661 82. 553 661 82. 553 661 82. 782 661 82. 035 661 82. 782 661 82. 035 661 82. 035 661 82. 035 662 92. 239 62 90. 411 62 91. 225 62 92. 049 62 93. 379 62 94. 168 62 91. 522 62 92. 297 62 93. 620 62 94. 395 62 94. 395 63 93. 192 63 93. 961 63 93. 961 63 95. 093 64 94. 565	43. 278 22. 23 41. 825 23. 93 46. 833 26. 13 47. 769 25. 33 46. 960 27. 45 48. 258 27. 93 48. 119 29. 16 47. 597 28. 83 46. 548 29. 65 47. 629 27. 58 47. 629 27. 58 46. 581 28. 36 47. 629 27. 58 48. 355 28. 78 49. 045 28. 46 50. 266 28. 55 48. 355 28. 78 49. 060 29. 28 48. 182 30. 24 49. 021 31. 18 48. 699 31. 46 49. 531 32. 25 50. 194 31. 73 51. 030 32. 52 50. 699 32. 77 51. 549 33. 53 49. 615 28. 18 49. 337 26. 99 50. 405 28. 56 51. 026 27. 58 52. 192 28. 23 51. 741 29. 15 52. 327 30. 24 50. 836 28. 78 50. 076 26. 85	79	(Continued) B O B O B O B O B O B O B C B C B C B C
ATOM 11109 ATOM 11111 ATOM 11111 ATOM 11112	N SER 6	63 94. 565 64 94. 453 64 95. 321 64 95. 464	49. 045 27. 37 50. 444 25. 61 49. 658 24. 73 50. 364 23. 39	2 1.00 13.86 8 1.00 13.65	B O B N B C
ATOM 11113 ATOM 11114 ATOM 11115	OG SER 60 C SER 60 O SER 60	64 96. 055 64 96. 714 64 97. 066	51. 642 23. 55 49. 340 25. 27 48. 176 25. 43	0 1.00 16.79 8 1.00 13.42 8 1.00 12.83	B C B C B C
ATOM 11116 ATOM 11117 ATOM 11118 ATOM 11119	CA VAL 60	65 97. 503 65 98. 865 65 99. 547 65 101. 023	50. 371 25. 55 50. 158 26. 04 51. 496 26. 42 51. 263 26. 66	1 1.00 15.86 7 1.00 14.66	B N B C B C B C
ATOM 11120 ATOM 11121 ATOM 11122	CG2 VAL 66 C VAL 66 O VAL 66	99. 354 99. 020	52. 519 25. 32 49. 169 27. 20 48. 400 27. 24	7 . 1. 00 15. 28 6 1. 00 15. 25	B C B C B O

					FIC	G. 4-	228			(Continued)
ATOM	11123	N	TYR	666	98. 091	49. 184	28. 154	1.00 17.07	В	N
ATOM	11124	CA	TYR	666	98.175	48. 276	29. 299	1.00 15.32	В	C
ATOM	11125	CB	TYR	666	97. 504	48. 896	30. 531 31. 751	1.00 13.28	B B	C .
ATOM ATOM	11126 11127	CD1	TYR TYR	666 666	97. 483 96. 595	47. 997 46. 920	31. 845	1.00 12.79 1.00 12.27	В	C
ATOM	11128		TYR	666	96. 583	46. 089	32. 964	1.00 12.21	В	Č
ATOM	11120		TYR	666	98. 360	48. 215	32. 809	1.00 12.00	В	Č
ATOM	11130			666	98. 361	47. 390	33. 928	1.00 12.03	В	Č
ATOM	11131	CZ	TYR	666	97. 472	46. 332	34.005	1.00 13.90	В	č
ATOM	11132	OH	TYR	666	97. 471	45. 531	35. 131	1.00 12.51	B	ŏ
ATOM	11133	Č	TYR	666	97. 550	46. 922	29. 023	1.00 15.26	B	Č
ATOM	11134	Ŏ	TYR	666	98. 103	45. 895	29. 399	1.00 18.30	B	Ö
ATOM	11135	N	THR	667	96. 401	46.912	28. 365	1.00 14.70	B	N
ATOM	11136	CA	THR	667	95. 712	45.656	28.097	1.00 13.70	В	C
ATOM	11137	CB	THR	667	94.264	45. 925	27.656	1.00 12.07	В	C
ATOM	11138	0G1	THR	667	93.617	46.756	28.635	1.00 11.17	В	0
ATOM	11139	CG2	THR	667	93. 498	44.624	27. 533	1.00 10.21	В	C
ATOM	11140	C	THR	667	96.423	44. 792	27.067	1.00 15.29	В	C
ATOM	11141	0	THR	667	96. 713	43.626	27. 323	1.00 16.16	В	0
ATOM	11142	N	GLU	668	96. 707	45. 372	25. 906	1.00 16.99	В	N
ATOM	11143	CA	GLU	668	97. 389	44.672	24. 823	1.00 16.90	В	C
ATOM	11144	CB	GLU	668	97. 537	45.612	23.625	1.00 17.50	В	C
ATOM	11145	CG	GLU	668	96. 231	45.808	22.867	1.00 21.31	В	C
ATOM	11146	CD	GLU	668	96. 275	46.928	21.850	1.00 22.06	В	C
ATOM	11147		GLU	668	97. 284	47.054	21.123	1.00 25.39	В	0
ATOM	11148		GLU	668	95. 284	47.679	21.767	1.00 22.03	В	0
ATOM ATOM	11149 11150	C	GLU GLU	668 668	98. 751	44. 127	25. 247	1.00 17.77	В	C
ATOM	11151	O N	ARG	669	99. 186 99. 418	43. 079 44. 827	24. 766 26. 158	1.00 19.28 1.00 17.62	В	0
ATOM	11151	CA	ARG	669	100. 721	44. 392	26. 640	1.00 17.02	B B	N C
ATOM	11153	CB	ARG	669	101. 199	45. 291	27. 785	1.00 17.00	В	Č
ATOM	11154	CG	ARG	669	102. 498	44. 828	28. 451	1.00 15.11	В	Č
ATOM	11155	CD	ARG	669	102. 878	45.766	29. 583	1.00 15.35	B	Č
ATOM	11156	NE	ARG	669	102. 914	47. 149	29. 122	1.00 16.25	В	N
ATOM	11157	CZ	ARG	669	102.549	48. 196	29. 856	1.00 16.96	В	Č
ATOM	11158	NH1	ARG	669	102.115	48. 023	31. 101	1.00 16.86	B	Ň
ATOM	11159		ARG	669	102.602	49.417	29. 340	1.00 14.86	B	N
ATOM	11160	C	ARG	669	100.633	42.960	27.140	1.00 17.70	B	Ċ
ATOM	11161	0	ARG	669	101.523	42.141	26.899	1.00 17.72	B	0
ATOM	11162	N	TYR	670	99. 539	42.655	27.825	1.00 17.60	В	N
ATOM	11163	CA	TYR	670	99. 357	41.333	28.385	1.00 16.56	В	С
ATOM	11164	CB	TYR	670	98. 823	41.465	29.810	1.00 15.82	В	C
ATOM	11165	CG	TYR	670	99.571	42.491	30.631	1.00 15.47	В	C
ATOM	11166		TYR	670	98. 978	43.706	30. 973	1.00 14.06	В	С
ATOM	11167		TYR	670	99.680	44.676	31.676	1.00 14.36	В	С
ATOM	11168		TYR	670	100.894	42. 268	31.024	1.00 15.93	В	C
ATOM	11169		TYR	670	101.608	43. 232	31. 732	1.00 15.78	В	C
ATOM	11170	CZ	TYR	670	100. 998	44. 433	32.051	1.00 15.30	В	С
ATOM	11171	OH	TYR	670	101.713	45. 403	32. 714	1.00 15.22	В	0

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(Continued)

					FIC	G. 4-	2 2 9			Continue
ATOM ATOM	11172 11173	C 0	TYR TYR	670 670	98. 435 98. 637	40. 441 39. 231	27. 578 27. 508	1.00 17.87 1.00 18.02	B B	C 0
ATOM	11174	N	MET	671	97. 435	41.040	26. 948	1.00 18.57	В	N
ATOM	11175	CA	MET	671	96. 452	40. 271	26. 199	1.00 10.01	В	Ċ
ATOM	11176	CB	MET	671	95.063	40.844	26. 482	1.00 21.47	B	č
ATOM	11177	CG	MET	671	94.604	40. 692	27. 919	1.00 21.74	B	č
ATOM	11178	SD	MET	671	94. 228	38. 972	28. 277	1.00 28.61	B	Š
ATOM	11179	CE	MET	671	92. 570	38. 871	27. 582	1.00 23.84	B	č
ATOM	11180	C	MET	671	96. 640		24. 692	1.00 19.95	B	Č
ATOM	11181	ŏ	MET	671	96. 121	39. 240	24. 075	1.00 20.85	В	0
ATOM	11182	Ň	GLY	672	97. 380	41.092	24.094	1.00 20.28	В	N
ATOM	11183	CA	GLY	672	97.540	41.063	22.654	1.00 19.08	В	С
ATOM	11184	C	GLY	672	96.354	41.807	22.068	1.00 21.12	В	С
ATOM	11185	Ö	GLY	672	95.746	42.629	22.755	1.00 21.18	В	0
ATOM	11186	N	LEU	673	96.009	41.534	20.814	1.00 21.68	В	N
ATOM	11187	CA	LEU	673	94. 884		20.186	1.00 21.44	В	С
ATOM	11188	CB	LEU	673	95. 204	42.569	18.732	1.00 22.03	В	C.
ATOM	11189	CG	LEU	673	96. 287	43.627	18.507	1.00 24.89	В	С
ATOM	11190	CD1	LEU	673	96. 518	43.837	17.023	1.00 23.45	В	C.
ATOM	11191	CD2	LEU	673	95. 846	44:932	19.150	1.00 27.67	В	C
ATOM	11192	C	LEU	673	93.616	41.399	20. 243	1.00 21.68	В	С
ATOM	11193	0	LEU	673	93. 647	40. 173	20.076	1.00 21.49	В	0
ATOM	11194	N	PR0	674	92. 475	42.061		1.00 21.61	В	N
ATOM	11195	CD	PR0	674	92. 342	43. 487	20.830	1.00 20.79	В	C C C
ATOM	11196	CA	PR0	674	91.180	41.388	20. 571	1.00 20.99	В	C
ATOM	11197	CB	PR0	674	90. 365	42. 347	21.420	1.00 19.09	В	C
ATOM	11198	CG	PR0	674	90. 845	43.664	20.941	1.00 18.24	В	C
ATOM	11199	C	PR0	674	90. 589	41. 155	19. 183	1.00 21.53	В	C
ATOM	11200	0	PR0	674	89. 470	41.561	18.884	1.00 20.30	В	0
ATOM	11201	N	THR	675	91.378	40. 505	18. 335	1.00 23.61	В	N
ATOM	11202	CA	THR	675	90. 973	40. 176	16.975	1.00 23.43	В	C
ATOM	11203	CB	THR	675	92. 045	40. 560	15.957	1.00 22.99	В	C
ATOM	11204	0G1			93. 221	39. 783	16. 200	1.00 24.15	В	0
ATOM	11205		THR	675	92.386	42.039	16.062	1.00 21.26	В	C
ATOM ATOM	11206 11207	C	THR	675	90. 825	38.668	16.931	1.00 25.46	В	C
ATOM	11207	O N	THR PRO	675 676	91.424	37. 952	17. 736	1.00 25.82	В	0 N
	11200				90. 023 89. 130	38. 160	15.991	1.00 26.60	В	N
ATOM	11210	CA	PRO	676	89. 823			1.00 25.76	В	
ATOM	11211	CB	PRO	676	88. 860	36. 714 36. 599	15. 877 14. 702	1.00 26.64 1.00 25.84	B B	C C
ATOM	11211	CG	PRO	676	88. 066	37. 859	14. 702	1.00 23.84	В	C
ATOM	11213	C	PRO	676	91.135	35. 967	15.630	1.00 24.33	В	C
ATOM	11214	ŏ	PRO	676	91.347	34. 875	16.160	1.00 28.85	В	0
ATOM	11215	Ň	GLU	677	92. 021	36. 557	14.834	1.00 30.55	В	N.
ATOM	11216	CA	GLU	677	93. 286	35. 905	14. 534	1.00 30.33	В	C
ATOM	11217	CB	GLU	677	93. 772	36. 290	13: 135	1.00 31.34	В	Č
ATOM	11218	CG	GLU	677	94. 177	35. 077	12. 294	1.00 33.44	В	Č
ATOM	11219	CD	GLU	677	92. 984	34. 204	11.897	1. 00 41. 70	В	C
ATOM	11220	0E1		677	92. 234	34. 610	10. 980	1. 00 49. 52	В	0
111 0111	11440	ODI	OHU	011	54.404	04.010	10.000	1.00 40.04	ע	U

										(Continued)
					FIG.	4 -	2 3 0			(Continued)
ATOM	11221	0E2	GLU	677	92. 789	33. 121	12. 503	1.00 46.47	В	0
ATOM	11222	C	GLU	677		36. 174	15.563	1.00 31.51	В	C
ATOM	11223	0	GLU	677		35. 938	15.305	1.00 31.18	В	0
ATOM	11224	N	ASP	678			16.730	1.00 29.04	В	N
ATOM	11225	CA	ASP	678		36. 896	17. 756	1.00 26.71	В	C
ATOM	11226	CB	ASP	678		38. 374	17. 917	1.00 25.30	В	C
ATOM	11227	CG	ASP	678		38. 586	18. 902	1.00 26.53	. B	C
ATOM	11228		ASP	678		39. 721 37. 612	19. 008 19. 579	1.00 29.18 1.00 24.47	В	0
ATOM	11229	C	ASP ASP	678 678		36. 325	19. 098	1.00 25.24	В	Č
ATOM ATOM	11230 11231	0	ASP	678		35. 200	19. 426	1.00 26.23	В	· ŏ
ATOM	11232	N	ASN	679		37. 082	19. 871	1.00 24.14	B	Ň
ATOM	11233	ČA	ASN	679		36.608	21.186	1.00 22.47	B	Ċ
ATOM	11234	CB	ASN	679		37. 089	22. 217	1.00 23.05	В	C
ATOM	11235	CG	ASN	679		36. 323	23.524	1.00 22.50	В	C
ATOM	11236	0D1	ASN	679		36.880	24. 592	1.00 21.44	В	0
ATOM	11237	ND2	ASN	679		35. 037	23. 448	1.00 22.30	В	N
ATOM	11238	С	ASN	679		37. 061	21.596	1.00 21.85	В	C
MOTA	11239	0	ASN	679		37. 174	22. 785	1.00 21.56	В	0
ATOM	11240	N	LEU	680		37. 316	20. 619	1.00 22.96	В	N
ATOM	11241	CA	LEU	680		37. 750	20. 913	1.00 22.05	В	C
ATOM	11242	CB	LEU	680		37. 967 38. 379	19. 617 19. 734	1.00 20.94 1.00 20.98	B B	C C
ATOM ATOM	11243 11244		LEU LEU	680 680		39. 671	20. 539	1.00 20.38	В	Č
ATOM	11244		LEU	680		38. 567	18. 348	1.00 17.15	В	č
ATOM	11246	C	LEU	680		36. 762	21. 805	1.00 22.36	B	č
ATOM	11247	ŏ	LEU	680		37. 171	22. 718	1.00 23.81	B	Ŏ
ATOM	11248	Ň	ASP	681		35. 466	21.555	1.00 22.95	В	N
ATOM	11249	CA	ASP	681		34. 469	22. 371	1.00 24.27	В	C
ATOM	11250	CB	ASP	681		33. 048	21.980	1.00 24.73	В	С
ATOM	11251	CG	ASP	681		32. 587	20.695	1.00 25.98	В	С
ATOM	11252		ASP	681		33. 334	20. 116	1.00 28.21	В	0
ATOM	11253		ASP	681		31. 462	20. 259	1.00 28.60	В	0
ATOM	11254	C	ASP	681		34. 655	23. 862	1.00 23.99	В	C
ATOM	11255	0	ASP	681		34. 640	24.660	1.00 24.77	В	0 at
ATOM	11256	N	HIS	682		34. 819	24. 252	1.00 22.66	В	N C
ATOM	11257	CA	HIS	682 682		34. 998 34. 867	25. 667 25. 981	1. 00 22. 62 1. 00 23. 03	B B	C C
ATOM ATOM	11258 11259	CB CG	HIS HIS	682		34. 898	27. 448	1.00 25.79	В	Č
ATOM	11260		HIS	682		35. 718	28. 190	1.00 26.73	В	Č
ATOM	11261		HIS	682		34. 035	28. 338	1.00 25.30	В	Ň
ATOM	11262		HIS	682		34. 326	29. 565	1.00 26.50	B	ĉ
ATOM	11263		HIS	682		35. 344	29. 504	1.00 26.09	B	N
ATOM	11264	C	HIS	682		36. 344	26. 175	1.00 21.71	B	Ċ
ATOM	11265	0	HIS	682		36. 465	27. 345	1.00 20.98	В	0
ATOM	11266	N	TYR	683		37. 355	25. 307	1.00 19.91	В	N
ATOM	11267	CA	TYR	683		38. 657	25. 707	1.00 19.50	В	C
ATOM	11268	CB	TYR	683		39. 646	24. 542	1.00 16.55	В	C
MOTA	11269	CG	TYR	683	90.419	40. 574	24. 472	1.00 16.85	В	C

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										(Continue	·4)
					FIG	. 4 -	2 3 1			(Oommad	,u,
ATOM	11970	CD1	TVD	600	01 616	40. 172	23. 877	1.00 16.	29 B	С	
ATOM ATOM	11270 11271		TYR TYR	683 683	91.616 92.700	41.040	23. 786	1.00 16.			
ATOM	11272		TYR	683	90. 345	41.871	24. 980	1.00 16.		Č	
ATOM	11273		TYR	683	91.430	42.748	24.893	1.00 14.		С	
ATOM	11274	CZ	TYR	683	92.598	42.326	24. 295	1.00 15.		C	
ATOM	11275	OH	TYR	683	93.663	43. 193	24. 192	1.00 16.		0	
ATOM	11276	C	TYR	683	87. 793	38. 437	26. 150	1.00 21.		C	
ATOM	11277	0	TYR	683	87.355	38. 955	27. 174	1.00 20.		0	
ATOM	11278	N	ARG ARG	684 684	87. 071 85. 667	37. 644 37. 349	25. 367 25. 634	1.00 22. 1.00 24.		N C	
ATOM ATOM	11279 11280	CA CB	ARG	684	84. 992	36. 871	24. 344	1.00 24.		Č	
ATOM	11281	CG	ARG	684	84. 996	37. 908	23. 234	1.00 25.		Č	
ATOM	11282	CD	ARG	684	84. 197	39. 132	23. 639	1.00 25.		Č	
ATOM	11283	NE	ARG	684	84.453	40.275	22.767	1.00 27.		N	
ATOM	11284	CZ	ARG	684	84. 126	40.344	21.480	1.00 27.		С	
ATOM	11285		ARG	684	83. 518	39. 327	20. 880	1.00 27.		N	
ATOM	11286		ARG	684	84.409	41.443	20. 794	1.00 26.		N	
ATOM	11287	C	ARG	684	85.401	36. 340	26. 745	1.00 24.		C	
ATOM ATOM	11288 11289	O N	ARG ASN	684 685	84. 275 86. 421	36. 239 35. 591	27. 231 27. 148	1.00 26. 1.00 24.		O N	
ATOM	11209	CA	ASN	685	86. 243	34. 593	28. 201	1.00 24.		C	
ATOM	11291	CB	ASN	685	86. 959	33. 294	27. 823	1.00 26.		Č	
ATOM	11292	CG	ASN	685	86. 132	32. 430	26. 904	1.00 33.		č	
ATOM	11293		ASN	685	85.076	31.924	27. 296	1.00 35.		0	
ATOM	11294		ASN	685	86.594	32. 260	25.667	1.00 36.		N	
ATOM	11295	C	ASN	685	86.716	35.043	29. 575	1.00 20.		C	
ATOM	11296	0	ASN	685	86.472	34. 361	30. 566	1.00 20.		0	
ATOM ATOM	11297 11298	N	SER	686	87. 382 87. 887	36.186	29.644	1.00 16.		N	
ATOM	11290	CA CB	SER SER	686 686	89. 360	36. 666 37. 063	30. 918 30. 773	1.00 16. 1.00 17.		C C	
ATOM	11300	OG	SER	686	89. 530	38.050	29. 768	1.00 17.		Ö	
ATOM	11301	Č	SER	686	87. 089	37. 837	31. 486	1.00 15.		č	
ATOM	11302	Õ	SER	686	87.625	38.667	32. 221	1.00 13.		Ö	
ATOM	11303	N	THR	687	85.807	37.905	31.155	1.00 14.		N	
ATOM	11304	CA	THR	687	84. 989	38. 992	31.655	1.00 15.		C	
ATOM	11305	CB	THR	687	83. 899	39,401	30.639	1.00 16.		C	
ATOM	11306	0G1		687	82. 915	38. 362	30, 537	1.00 18.		0	
ATOM ATOM	11307 11308	C	THR THR	687 687	84. 519 84. 309	39. 657 38. 605	29. 265 32. 957	1.00 16. 1.00 14.		C C	
ATOM	11309	ŏ	THR	687	84. 153	37. 425	33. 264	1.00 14.		0	
ATOM	11310	N	VAL	- 688	83. 910	39. 616	33. 717	1.00 14.		N	
ATOM	11311	ĊA	VAL	688	83. 224	39. 411	34. 977	1.00 14.		C	
ATOM	11312	CB ·	VAL	688	83. 239	40.691	35. 824	1.00 15.	57 B	С	
ATOM	11313	CG1		688	82. 476	40.464	37. 130	1.00 15.		C	
ATOM	11314		VAL	688		41.115	36. 100	1.00 18.		C	
ATOM	11315	C	VAL	688	81.777	39.048	34. 687	1.00 14.		C	
ATOM	11316	0 N	VAL	688	81. 196	38. 188	35. 350	1.00 15.		0	
ATOM	11317 11318	N CA	MET MET	689 680	81.209	39.710	33. 682 33. 283	1.00 13.1 1.00 14.		N C	
ATOM	11910	UM	iiii; I	689	79. 826	39. 496	00. 400	1.00 14.	io D	U	

F I G. 4 - 232	Continued)
FIG. 4 - 232 ATOM 11319 CB MET 689 79.519 40.287 32.010 1.00 14.10 B GATOM 11320 CG MET 689 79.359 41.793 32.217 1.00 18.18 B GATOM 11321 SD MET 689 80.817 42.684 32.849 1.00 21.67 B SATOM 11322 CE MET 689 81.693 43.067 31.308 1.00 19.11 B GATOM 11323 C MET 689 79.429 38.040 33.080 1.00 13.66 B GATOM 11324 O MET 689 78.398 37.597 33.586 1.00 14.01 B GATOM 11325 N SER 690 80.246 37.290 32.356 1.00 14.32 B ATOM 11326 CA SER 690 79.939 35.887 32.087 1.00 16.68 B GATOM 11327 CB SER 690 81.018 35.259 31.199 1.00 18.28 B GATOM 11328 OG SER 690 82.225 35.062 31.923 1.00 23.11 B GATOM 11329 C SER 690 79.771 35.019 33.328 1.00 15.55 B GATOM 11330 O SER 690 79.212 33.927 33.234 1.00 16.21 B GATOM 11331 N ARG 691 80.238 35.502 34.478 1.00 16.21 B GATOM 11332 CA ARG 691 80.238 35.502 34.478 1.00 14.35 B GATOM 11333 CB ARG 691 80.155 34.741 35.727 1.00 15.38 B GATOM 11333 CB ARG 691 80.155 34.741 35.727 1.00 15.38 B GATOM 11333 CB ARG 691 80.155 34.741 35.727 1.00 15.38 B GATOM 11333 CB ARG 691 80.155 34.741 35.727 1.00 15.38 B GATOM 11333 CB ARG 691 80.155 34.741 35.727 1.00 15.38 B GATOM 11334 CG ARG 691 82.697 34.414 35.652 1.00 19.96 B	
ATOM 11366 CB PHE 695 77.205 36.772 42.041 1.00 20.88 B C ATOM 11367 CG PHE 695 78.533 37.397 41.695 1.00 19.06 B C	

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(Continued)

F	T	G.	4 -	2	3	3
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ATOM	11368	CD1	PHE	695	79. 211	37.042	40.533	1.00 19.50	В	С
ATOM	11369		PHE	695	79.096	38. 365	42.523	1.00 19.69	B	Č
ATOM	11370		PHE	695	80. 431	37. 647	40. 200	1.00 18.29	B	Č
ATOM	11371		PHE	695	80. 316	38. 977	42. 199	1.00 18.53	В	Č
ATOM	11372	CZ	PHE	695	80. 982	38. 615	41.033	1.00 17.35	В	Č
ATOM	11372	C	PHE	695	76. 146	35. 052	43. 483	1.00 14.33	В	Č
ATOM	11373	Ö	PHE	695	76. 090	35. 636	44. 566	1.00 24.37	В	0
ATOM	11375	N	LYS	696	75. 230	34. 173	43. 089	1.00 23.07	В	N
ATOM	11376	CA	LYS	696	74. 074	33. 880	43. 926	1.00 24.40	В	C
ATOM	11377	CB	LYS	696	73. 173	32. 813	43. 280	1.00 23.82	В	C
ATOM	11378	CG	LYS	696	72. 076	32. 281	44. 228	1.00 21.13	В	C
ATOM	11379	CD	LYS	696	70. 680	32. 287	43.615	1.00 30.02	В	C
ATOM	11380	CE	LYS	696	70. 137	33. 705	43. 421	1.00 31.03	В	Č
ATOM	11381	NZ	LYS	696	69. 903	34. 438	44. 705	1.00 35.45	В	N
ATOM	11382	C	LYS	696	74. 402	33. 459	45.348	1.00 35.47	В	
ATOM	11383	0	LYS	696	73. 583	33. 641	46. 242	1.00 24.85	В	C
ATOM	11384	N	GLN	697	75. 587	32. 907	45. 577	1.00 24.94	В	0
ATOM	11385	CA	GLN	697	75. 920	32. 481	46. 931			N
ATOM	11386	CB	GLN	697	76.355				В	C
ATOM	11387	CG	GLN	697	75. 290	31.010	46.941 46.444	1.00 29.90	В	C
ATOM	11388	CD	GLN	697		30. 025		1.00 30.66	В	C
ATOM	11389	0E1	GLN		75.565	28. 593	46.889	1.00 30.92	В	C
				697	75.381	28. 245	48.065	1.00 31.54	В	0
ATOM	11390	NE2	GLN	697	76.019	27. 761	45.958	1.00 26.21	В	N
ATOM	11391	C	GLN	697	76.964	33. 322	47.662	1.00 26.04	В	C
ATOM	11392	0	GLN	697	77. 620	32. 833	48.580	1.00 28.31	В	0
ATOM	11393	N	VAL	698	77. 125	34. 580	47. 270	1.00 23.16	В	N
ATOM	11394	CA	VAL	698	78. 085	35. 445	47. 947	1.00 21.23	В	C
ATOM	11395	CB	VAL	698	79. 411	35. 596	47.156	1.00 20.63	В	Č
ATOM	11396	CG1	VAL	698	80. 033	34. 238	46. 901	1.00 17.19	В	C
ATOM	11397	CG2	VAL	698	79. 161	36. 335	45. 853	1.00 18.36	В	Č
ATOM	11398	C	VAL	698	77. 496	36. 829	48. 118	1.00 21.50	В	C
ATOM	11399	0	VAL	698	76. 571	37. 207	47.404	1.00 23.06	В	0
ATOM	11400	N	GLU	699	78.018	37. 579	49.078	1.00 21.31	В	N
ATOM	11401	CA	GLU	699	77.563	38. 945	49. 290	1.00 21.42	В	Č
ATOM	11402	CB	GLU	699	77. 465	39. 246	50. 785	1.00 22.73	В	C
ATOM	11403	CG	GLU	699	76.396	38. 403	51.461	1.00 26.07	В	C
ATOM	11404	CD	GLU	699	76.547	38. 346	52.961	1.00 29.09	В	C
ATOM	11405	0E1	GLU	699	76.343	39. 387	53.624	1.00 31.29	В	0
ATOM	11406	0E2		699	76.876	37. 254	53.476	1.00 31.07	В	0
ATOM	11407	C	GLŲ	699	78.610	39.810	48. 593	1.00 21.23	В	C
ATOM	11408	0	GLU	699	79.802	39. 751	48. 905	1.00 21.45	В	0
ATOM	11409	N	TYR	700	78. 148	40. 594	47.630	1.00 19.47	В	N
ATOM	11410	CA	TYR	700	79.012	41. 428	46.818	1.00 18.26	В	C
ATOM	11411	CB	TYR	700	78. 830	41.001	45. 368	1.00 18.24	В	С
ATOM	11412	CG	TYR	700	79.678	41.685	44. 330	1.00 18.56	В	C
ATOM	11413		TYR	700	81.071	41.698	44.422	1.00 17.75	В	C
ATOM	11414	CE1		700	81.856	42.206	43. 378	1.00 17.99	В	С
ATOM	11415	CD2		700	79.088	42. 209	43. 181	1.00 19.07	В	C
ATOM	11416	CE2	TYR	700	79.852	42.715	42. 143	1.00 19.54	В	C

				F I G. 4 - 234	(Continued)
ATOM	11417	CZ TYR	700	81. 231 42. 707 42. 241 1. 00 19. 61 B	С
ATOM	11418	OH TYR	700	81.964 43.170 41.176 1.00 20.17 B	0
ATOM	11419	C TYR	700	78. 697 42. 902 46. 972 1. 00 18. 20 B	C
ATOM	11420	0 TYR	700	77. 534 43. 288 47. 006 1. 00 19. 67 B	0
ATOM	11421	N LEU	701	79. 748 43. 714 47. 078 1. 00 16. 71 B	N
ATOM	11422	CA LEU	701	79. 628 45. 157 47. 198 1. 00 15. 24 B	C
ATOM	11423	CB LEU	701	80. 102 45. 624 48. 573 1. 00 14. 82 B	C
ATOM	11424	CG LEU	701	80. 195 47. 141 48. 768 1. 00 15. 42 B	C
ATOM	11425	CD1 LEU	701	78. 926 47. 810 48. 280 1. 00 16. 37 B	C
ATOM	11426	CD2 LEU	701	80.449 47.456 50.233 1.00 13.32 B	C C
ATOM	11427	C LEU	701 701	80. 491 45. 770 46. 095 1. 00 16. 15 B 81. 714 45. 617 46. 082 1. 00 16. 12 B	0
ATOM ATOM	11428 11429	O LEU N LEU	702	79. 829 46. 450 45. 167 1. 00 14. 91 B	N
ATOM	11429	CA LEU	702	80.467 47.073 44.019 1.00 13.94 B	Č
ATOM	11431	CB LEU	702	79. 730 46. 627 42. 753 1. 00 15. 12 B	č
ATOM	11432	CG LEU	702	80.119 47.175 41.383 1.00 15.68 B	č
ATOM	11433	CD1 LEU	702	81.555 46.814 41.050 1.00 14.64 B	C C
ATOM	11434	CD2 LEU	702	79.173 46.593 40.354 1.00 16.45 B	Ċ
ATOM	11435	C LEU	702	80.419 48.590 44.169 1.00 14.21 B	C
ATOM	11436	0 LEU	702	79. 346 49. 166 44. 314 1. 00 14. 96 B	0
ATOM	11437	N ILE	703	81. 591 49. 220 44. 132 1. 00 13. 90 B	N
ATOM	11438	CA ILE	703	81.737 50.662 44.294 1.00 13.91 B	C
ATOM	11439	CB ILE	703	82. 543 50. 967 45. 578 1. 00 13. 87 B	C
ATOM	11440	CG2 ILE	703	82. 693 52. 491 45. 775 1. 00 15. 37 B	C
ATOM	11441	CG1 ILE	703	81. 869 50. 308 46. 782 1. 00 12. 11 B	C
ATOM	11442	CD1 ILE	703	82. 714 50. 328 48. 047 1. 00 7. 95 B	C
ATOM	11443	C ILE	703	82. 495 51. 251 43. 101 1. 00 15. 43 B	C
ATOM	11444	O ILE N HIS	703 704	83. 379 50. 600 42. 548 1. 00 17. 12 B 82. 175 52. 484 42. 714 1. 00 14. 44 B	O N
ATOM ATOM	11445 11446	N HIS CA HIS	704	82. 175 52. 484 42. 714 1. 00 14. 44 B 82. 866 53. 098 41. 579 1. 00 14. 11 B	C
ATOM	11447	CB HIS	704	82. 483 52. 356 40. 288 1. 00 12. 85 B	č
ATOM	11448	CG HIS	704	83. 539 52. 386 39. 224 1. 00 13. 44 B	č
ATOM	11449	CD2 HIS	704	84. 363 53. 377 38. 806 1. 00 12. 54 B	č
ATOM	11450	ND1 HIS	704	83. 827 51. 293 38. 435 1. 00 12. 00 B	Ň
ATOM	11451	CE1 HIS	704	84. 782 51. 607 37. 578 1. 00 10. 09 B	C
ATOM	11452	NE2 HIS	704	85. 125 52. 865 37. 782 1. 00 12. 68 B	N ·
ATOM	11453	C. HIS	704	82. 533 54. 584 41. 457 1. 00 13. 37 B	C
ATOM	11454	0 HIS	704	81. 420 55. 007 41. 770 1. 00 15. 67 B	0
ATOM	11455	N GLY	705	83. 513 55. 372 41. 027 1. 00 10. 99 B	N
ATOM	11456	CA GLY	705	83. 308 56. 798 40. 860 1. 00 10. 39 B	C
ATOM	11457	C GLY	705	82. 807 57. 082 39. 457 1. 00 10. 13 B	C
ATOM	11458	0 GLY	705	83. 326 56. 536 38. 483 1. 00 11. 85 B	0
ATOM	11459	N THR	706	81. 805 57. 942 39. 347 1. 00 10. 36 B	N
ATOM	11460	CA THR	706	81. 215 58. 272 38. 054 1. 00 9. 96 B	C
ATOM ATOM	11461	CB THR OG1 THR	706 706	79. 935 59. 072 38. 232 1. 00 6. 56 B 80. 251 60. 367 38. 739 1. 00 8. 64 B	C 0
ATOM	11462 11463	CG2 THR	706 706	80. 251 60. 367 38. 739 1. 00 8. 64 B 79. 025 58. 372 39. 215 1. 00 8. 26 B	C
ATOM	11464	CGZ THR	706	82. 145 59. 052 37. 147 1. 00 11. 88 B	C
ATOM	11465	0 THR	706	81. 994 59. 018 35. 927 1. 00 13. 83 B	0
tri On	11100	2 1111	100	01. 337 03. 010 00. 021 1. 00 10. 00 D	U

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(Continued) FIG. 4-235 37.739 ATOM 11466 707 83.114 59.741 1.00 13.21 N N ALA 36.969 84.075 60.5221.00 14.57 C ATOM 11467 707 В CA ALA 11468 84.277 61.881 37.626 1.00 17.64 ATOM CB ALA 707 B 36.802 11469 85.427 59.823 1.00 13.77 C C В ATOM ALA 707 60.484 1.00 14.15 86.445 36.639 11470 707 0 ATOM 0 ALA 36.839 ATOM 11471 N **ASP** 708 85.435 58.494 1.00 13.35 В N 86.667 57.721 36.685 ATOM 11472 CA **ASP** 708 1.00 12.65 B C 56. 285 55. 536 11473 86.439 37.188 1.00 12.24 ATOM CB ASP 708 B C 87.737 ATOM 11474 37.453 1.00 10.05 В CG ASP 708 ATOM 11475 OD1 ASP 708 88.738 55.775 36.749 1.00 11.19 В 0 ATOM 11476 OD2 ASP 87.751 54.686 38.362 1.00 9.31 В 0 708 87.091 35. 202 11477 57.696 1.00 13.18 В ATOM C ASP 708 ATOM 11478 ASP 86.475 57.023 1.00 13.78 В 0 708 34.368 0 **ATOM** 11479 ASP 88.156 58.423 34.891 N 709 1.00 12.80 В N 88.679 58.520 **ATOM** 11480 ASP 709 33.534 1.00 12.65 CA В C 11481 **ASP** 59.825 ATOM 89.442 33.397 C CB 709 1.00 11.74 В ATOM 90.612 C CG **ASP** 59.912 34.366 11482 709 1.00 9.63 B **ATOM** 11483 OD1 ASP 91.704 59.385 34.058 2.39 709 1.00 В 0 ATOM 11484 OD2 ASP 90.419 60.499 35.451 0 709 1.00 11.84 В 89.605 11485 ASP 57.366 33.167 C ATOM C 709 1.00 14.57 ATOM 11486 **ASP** 89.896 57.136 0 709 31.987 1.00 16.47 В 0 ATOM 11487 ASN 90.076 56.652 34.182 N 710 1.00 13.58 В N **ATOM** 11488 ASN 90.981 55.524 33.990 1.00 13.56 CA 710 В C ASN 55.385 Č ATOM 11489 91.841 CB 710 35.243 1.00 13.26 В ATOM 11490 CG ASN 710 92.987 54.440 35.059 1.00 12.07 C В ATOM 11491 93.951 OD1 ASN 710 54.478 35.821 1.00 16.69 В 0 11492 ND2 ASN 92.898 53.578 ATOM 710 34.058 1.00 8.28 В N 11493 ATOM ASN 710 90.177 54.236 33.724 1.00 14.26 B C ATOM 11494 0 ASN 710 90.142 53.737 32.598 1.00 14.29 В 0 11495 89.560 ATOM N VAL 711 53.692 34.773 1.00 13.24 В N 88. 715 88. 835 52.511 ATOM 11496 CA VAL 34.652 1.00 12.56 711 В C ATOM 11497 CB VAL 51.585 35.868 1.00 11.72 711 В C ATOM 11498 CG1 VAL 88.048 711 50.311 35.624 1.00 7.36 В C 11499 ATOM CG2 VAL 90.287 51.274 36.141 711 1.00 13.94 В 11500 C ATOM VAL 87.315 711 53.119 34.645 1.00 14.01 В C 0 ATOM 11501 VAL 86.768 53.471 711 35.694 1.00 13.52 В 0 ATOM 11502 N HIS 86.746 53. 249 712 33.456 1.00 13.66 B N ATOM 11503 53.869 CA HIS 85.440 712 33.290 1.00 13.44 B C ATOM 11504 CB HIS 712 85.132 53.956 31.794 1.00 12.94 C В ATOM 11505 86.219 CG HIS 712 54.613 31.001 1.00 14.38 C В 87. 137 55.549 11506 ATOM CD2 HIS 712 31.352 1.00 15.50 В C 11507 ND1 HIS ATOM 712 86.477 54. 299 29.684 1.00 15.76 В N ATOM 11508 CE1 HIS 712 87.510 55.009 29.258 1.00 17.42 В C 87. 928 84. 293 11509 ATOM NE2 HIS 712 55.775 30.251 1.00 16.57 В N **ATOM** HIS 11510 C 712 53. 205 34.048 1.00 13.09 В C ATOM 11511 0 HIS 712 84.208 51.983 34.148 1.00 13.25 ATOM 11512 N PHE 713 83.420 54.041 1.00 13.27 34.594 В N **ATOM** 11513 CA PHE 713 82.253 53.586 35.335 1.00 15.36 C В

ATOM 11514 CB

PHE

713

81.288

54.759

SUBSTITUTE SHEET (RULE 26)

35.530

1.00 15.17

				FΙ	G. 4 -	2 3 6			(Continue	d)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	11515 11516 11517 11518 11519 11520 11521 11522 11523 11524 11525 11526 11527 11528 11529 11530 11531 11532 11533 11534 11535 11536 11537 11538	CD1 PICCE2 PICCE	HE 713 HE 713 HE 713 HE 713 HE 713 HE 713 LN 714 LN 714 LN 714 LN 714 LN 714 LN 714 LN 715 LN 715 LN 715 LN 715	80. 15 80. 34 78. 90 79. 30 77. 84 78. 05 81. 58 81. 01 81. 75 81. 69 82. 66 83. 82 82. 18 80. 51 82. 55 82. 56 84. 39 85. 27 86. 50 86. 47	6 54. 464 6 54. 508 1 54. 111 4 54. 204 8 53. 803 1 53. 849 6 52. 486 5 51. 527 3 52. 649 11 51. 699 13 51. 923 19 50. 703 11 51. 167 13 50. 493 14 50. 256 2 49. 389 449. 997 48. 646 15 48. 581 16 49. 086 17 48. 247 10 48. 889	36. 461 37. 841 35. 962 38. 710 36. 829 38. 204 34. 499 35. 031 33. 181 32. 228 30. 857 29. 946 28. 770 28. 943 27. 577 32. 650 32. 487 33. 192 33. 593 33. 926 32. 767 32. 537 32. 674 32. 155	1. 00 16. 61 1. 00 14. 51 1. 00 15. 42 1. 00 14. 71 1. 00 15. 24 1. 00 16. 62 1. 00 16. 48 1. 00 15. 73 1. 00 16. 08 1. 00 16. 13 1. 00 15. 37 1. 00 15. 37 1. 00 15. 37 1. 00 15. 35 1. 00 15. 29 1. 00 16. 29 1. 00 14. 60 1. 00 14. 55 1. 00 16. 01 1. 00 14. 28 1. 00 17. 54 1. 00 12. 78 1. 00 12. 78	B B B B B B B B B	CCCCCONCCONCCCCON	d)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	11539 11540 11541 11542 11543 11544 11545 11546 11551 11552 11553 11554 11555 11556 11557 11558 11560 11561 11562 11563	O G S S C S S C S S S C S S S S C S S S S		81. 61 81. 74 80. 88 81. 05 82. 27 79. 45 78. 68 77. 63 77. 40 77. 30 76. 21 78. 00 78. 00 78	.6 46. 967 .12 49. 002 .13 48. 602 .14 49. 544 .18 49. 295 .12 47. 692 .12 47. 692 .12 47. 693 .12 47. 696 .12 47. 682 .12 47. 682 .12 47. 682 .13 46. 214 .14 47. 232 .15 46. 319 .16 45. 235 .17 44. 248 .18 45. 320 .18 47. 278 .19 44. 226	34. 746 34. 749 35. 714 36. 829 38. 028 38. 700 36. 394 36. 814 35. 552 35. 083 34. 143 34. 382 34. 539 33. 623 32. 928 31. 858 30. 722 29. 691 30. 012 28. 449 33. 908 33. 695 34. 981 35. 953 37. 079	1.00 14.99 1.00 13.70 1.00 12.14 1.00 11.18 1.00 11.19 1.00 13.48 1.00 9.18 1.00 5.81 1.00 8.69 1.00 10.91 1.00 10.72 1.00 10.72 1.00 10.32 1.00 8.83 1.00 6.53 1.00 8.70 1.00 13.43 1.00 13.43 1.00 13.43 1.00 13.43 1.00 13.43 1.00 13.43 1.00 12.24 1.00 12.88	B B B B B B B B B B B B B B B B B B B	CONCCOCONCCCONCCONCC	

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							(Continued)
					FIG. 4-238		(002022
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	11613 11614 11615 11616 11617 11618 11620 11621 11622 11623 11624 11625 11626 11627 11628 11630 11631 11632 11633 11634 11635 11637 11638 11639	C O N CA CB CG OD1 OD2 C O N CA	VAL VAL GLY GLY VAL VAL VAL VAL VAL VAL VAL ASP ASP ASP ASP ASP PHE PHE	726 726 726 726 726 727 727 727 727 728 728 728 728 728 728	70. 409 36. 726 36. 329 1. 00 17. 93 71. 727 35. 920 36. 392 1. 00 19. 28 72. 246 35. 672 34. 994 1. 00 19. 33 72. 763 36. 660 37. 238 1. 00 19. 80 69. 789 36. 741 37. 723 1. 00 17. 35 69. 858 35. 756 38. 463 1. 00 16. 63 69. 198 37. 875 38. 081 1. 00 17. 14 68. 548 38. 012 39. 370 1. 00 15. 42 69. 387 37. 856 40. 626 1. 00 15. 90 68. 961 37. 182 41. 559 1. 00 17. 97 70. 568 38. 462 40. 675 1. 00 15. 07 71. 389 38. 357 41. 876 1. 00 14. 10 72. 859 37. 972 41. 574 1. 00 14. 97 73. 693 38. 145 42. 829 1. 00 13. 51 72. 954 36. 514 41. 109 1. 00 15. 40 71. 396 39. 687 42. 603 1. 00 14. 73 71. 738 40. 714 42. 025 1. 00 14. 56 71. 007 39. 672 <	B B B B B B B B B B B B B B B B B B B	Continued) C C C C C C C C C C C C C C C C C C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM	11632 11633 11634 11635 11636 11637 11638	CB CG OD1 OD2 C O N CA CB CG CD1 CD2 CE1	ASP ASP ASP ASP ASP PHE	729 729 729 729 729 729 730	70. 146 40. 731 45. 903 1. 00 15. 31 70. 034 42. 019 46. 696 1. 00 18. 11 69. 663 43. 055 46. 104 1. 00 20. 57 70. 317 42. 011 47. 907 1. 00 20. 06 72. 441 41. 185 45. 021 1. 00 16. 27 73. 253 40. 270 45. 117 1. 00 17. 70 72. 772 42. 454 45. 211 1. 00 16. 74 74. 136 42. 824 45. 579 1. 00 16. 43 75. 061 42. 734 44. 361 1. 00 13. 47 74. 744 43. 728 43. 304 1. 00 12. 81 75. 282 45. 006 43. 355 1. 00 12. 64 73. 828 43. 423 42. 303 1. 00 12. 46 74. 907 45. 966 42. 432 1. 00 11. 61 73. 446 44. 377 41. 376 1. 00 9. 11 73. 986 45. 653 41. 443 1. 00 10. 39 74. 112 44. 242 46. 114 1. 00 17. 87 73. 094 44. 928 46. 014 1. 00 19. 72 75. 230 44. 67	B B B B B	C C O C O N
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	11651 11652 11653 11654 11655 11656 11657 11658 11659 11660	CB CG CD OE1	GLN GLN GLN GLN GLN GLN ALA ALA ALA	731 731 731 731 731 731 731 732 732 732 732	76.089 45.961 48.569 1.00 18.02 75.547 44.948 49.536 1.00 25.59 74.087 45.183 49.854 1.00 29.48 73.699 46.275 50.281 1.00 31.32 73.263 44.157 49.647 1.00 32.13 76.124 46.889 46.272 1.00 16.69 77.060 46.417 45.623 1.00 13.71 75.737 48.158 46.172 1.00 15.59 76.425 49.084 45.284 1.00 15.79 75.718 49.147 43.946 1.00 15.47	B B B B B B B B B	C C C O N C O N C C

										(Cont.	inued)
					FIG	. 4 -	2 3 9			(00110	121404,
					1 1 0	•					
ATOM	11662	0	ALA	732		50. 897	46. 734	1.00 17.93	В	0	
ATOM	11663		MET	733		51.220	45. 382	1.00 17.27	В	N	
ATOM	11664	CA	MET	733		52.587	45.812	1.00 17.39	В	C	
ATOM	11665	CB	MET	733		52.628	47. 136	1.00 18.98	В	C	
ATOM	11666	CG	MET	733		54.028	47.661	1.00 18.20	В	C	
ATOM	11667	SD	MET	733		54. 979	47. 988	1.00 21.42	В	S	
ATOM	11668		MET	733		54. 324	49. 578	1.00 19.12	В	C	
ATOM	11669		MET	733		53. 268	44. 719	1.00 17.47	В	C	
ATOM	11670		MET	733		52. 783	44.318	1.00 17.30	В	0	
ATOM	11671	N	TRP	734	78.007	54. 378	44. 220	1.00 16.37	В	N	
ATOM	11672	CA	TRP	734		55. 147	43. 175	1.00 15.48	В	C	
ATOM	11673	CB	TRP	734		55. 428	42. 033	1.00 14.82	В	C C	
ATOM	11674	CG	TRP	734		56. 523	42. 353	1.00 14.06	В	C	
ATOM	11675	CD2		734		56.363	42.650	1.00 12.49	B B	C C	
ATOM	11676	CE2		734		57.645	42. 939	1.00 12.15	В	Č	
ATOM	11677	CE3		734	74. 437	55. 259	42. 701 42. 468	1.00 12.01 1.00 12.61	В	C	
ATOM	11678	CD1		734	76. 953	57. 857 58. 535	42. 408	1.00 12.01	В	Ň	
ATOM	11679	NE1		734	75.817	57. 858	43. 276	1.00 11.75	B.	Č	
ATOM	11680	CZ2		734		55. 466	43. 210	1.00 11.13	В		
ATOM	11681	CZ3		734	73. 115 72. 629	56. 762	43. 319	1.00 13.13	В	C C C	
ATOM	11682	CH2	TRP	734 734	79. 111	56. 457	43. 831	1.00 13.60	В	č	
ATOM	11683	C	TRP	734	78. 491	56. 881	44. 788	1.00 14.71	В	ő	
ATOM	11684 11685	O N	TYR	735	80. 174	57. 090	43. 346	1.00 13.31	B	Ň	
ATOM ATOM	11686	CA	TYR	735	80. 598	58. 366	43.926	1.00 12.17	B	Ċ	
ATOM	11687	CB	TYR	735	81.990	58. 260	44. 575	1.00 10.49	B	Č	
ATOM	11688	CG	TYR	735	81.964	57. 577	45. 920	1.00 10.18	B	Č	
ATOM	11689		TYR	735	81.464	58. 232	47.045	1.00 11.23	В	C	
ATOM	11690		TYR	735	81. 321	57. 567	48. 272	1.00 11.72	B	C	
ATOM	11691		TYR	735	82. 336	56. 241	46.052	1.00 11.30	В.	C	
ATOM	11692		TYR	735	82. 198	55. 567	47.270	1.00 11.75	В	С	
ATOM	11693	CZ	TYR	735	81.687	56. 235	48.372	1.00 12.02	В	С	
ATOM	11694	OH	TYR	735	81.511	55. 564	49.563	1.00 13.79	В	0	
ATOM	11695	C	TYR	735	80. 595	59.430	42.845	1.00 14.20	В	С	
ATOM	11696	0	TYR	735	81.391	59.393	41.910	1.00 15.56	В	0	
ATOM	11697	N	THR	736	79.669	60.372	42.977	1.00 15.66	В	N	
ATOM	11698	CA	THR	736	79. 517	61.459	42.026	1.00 14.01	В	C	
ATOM	11699	CB	THR	736	78. 395	62.401	42.469	1.00 13.01	В	С	•
ATOM	11700	0G1	THR	736	77. 163	61.673	42. 534	1.00 13.00	В	0	
ATOM	11701	CG2	THR	736	78. 256	63. 571	41.503	1.00 11.91	В	C	
ATOM	11702	C	THR	736	80. 789	62. 278	41.882	1.00 16.80	В	Ç	
ATOM	11703	0	THR	736	81.357	62.730	42.875	1.00 19.71	В	0	
ATOM	11704	N	ASP	737	81.230	62.457	40.640	1.00 16.82	В	N	
ATOM	11705	CA	ASP	737	82. 407	63. 257	40. 322	1.00 15.22	В	C	
ATOM	11706	CB	ASP	737	82. 151	64.728	40.684	1.00 15.24	В	C	
ATOM	11707	CG	ASP	737	81. 101	65. 380	39. 785	1.00 17.61	В	C	
ATOM	11708		ASP	737	80.697	64. 753	38. 779	1.00 16.59	В	0	
ATOM	11709		ASP	737	80.680	66. 525	40.078	1.00 19.23	В	0	
ATOM	11710	C	ASP	737	83. 737	62.811	40. 912	1.00 15.17	В	С	
								^.			

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(Continued) FIG. 4-241 49.390 63. 251 1.00 15.05 C 88.515 ATOM 11760 C SER 744 88.136 62.147 49.770 1.00 17.03 0 В ATOM 11761 0 SER 744 88. 822 64. 223 50.229 1.00 16.05 N 11762 В **ATOM** N SER 745 64.051 51.666 88.712 1.00 15.38 C 11763 B CA SER 745 ATOM 65.410 52.361 88.811 1.00 15.23 C 11764 SER В CB 745 ATOM 88. 357 65.318 53.698 1.00 20.36 0 ATOM 11765 0G SER 745 63.360 52.103 C 87.427 1.00 14.58 11766 B ATOM C SER 745 62.334 52.773 1.00 15.64 11767 87.467 В 0 **ATOM** 0 SER 745 86. 287 85. 009 63.925 51.728 1.00 13.39 **ATOM** 11768 THR В N N 746 63.355 52.121 1.00 12.46 **ATOM** 11769 THR 746 В C CA 64.299 1.00 13.02 ATOM 11770 CB THR 746 83.836 51.755 В C 83. 858 83. 929 11771 64.579 50.347 1.00 12.13 В 0 OG1 THR **ATOM** 746 CG2 THR 65.599 52.547 1.00 6.36 В C **ATOM** 11772 746 84.748 61.982 51.513 1.00 13.71 В ATOM 11773 746 C THR 11774 84.382 61.045 52.215 1.00 13.77 **ATOM** THR 746 В 0 0 84.948 11775 ALA 61.852 50.211 1.00 15.70 В **ATOM** 747 N N 84.698 60.575 1.00 17.75 11776 49.556 В C **ATOM ALA** CA 747 C 84.918 60.698 1.00 18.85 **ATOM** 11777 **ALA** 747 48.047 В CB 11778 85.579 50.133 1.00 16.94 C ATOM C **ALA** 747 59.482 В 11779 85.136 58.344 50.314 1.00 17.92 0 **ALA** В 0 ATOM 747 86.828 59.829 ATOM 11780 HIS 50.418 1.00 15.98 N N 748 87.772 58.873 **ATOM** 11781 CA HIS 748 50.987 1.00 15.53 С 51.194 ATOM 11782 CB HIS 89.130 59.547 1.00 14.50 C 748 В 51. 974 53. 124 11783 CG HIS 90.106 58.721 1.00 12.65 ATOM 748 В 90.772 11784 58.979 **ATOM** CD2 HIS 1.00 12.46 B 748 ND1 HIS ATOM 11785 90.517 57.472 51.566 1.00 11.91 В 748 N 56.998 11786 91.397 CE1 HIS 52.430 1.00 12.20 ATOM 748 В C 91. 569 87. 259 57.893 11787 NE2 HIS ATOM 748 53.384 1.00 9.44 В N 58.310 MOTA 11788 C HIS 748 52.316 1.00 15.00 В C 11789 HIS 87.272 57.097 ATOM 0 748 52.533 1.00 14.52 В 0 86. 808 86. 283 11790 1.00 14.63 ATOM N **GLN** 749 59.196 53.200 N В GLN 58.780 ATOM 11791 CA 54.496 1.00 15.23 749 В C ATOM 11792 CB GLN 749 86.045 59.999 55.378 1.00 15.87 C В ATOM 11793 87.314 60.722 Ċ CG GLN 749 55.740 1.00 22.62 B 87. 056 86. 511 61.956 Ċ ATOM 11794 CD GLN 1.00 25.83 749 56.564 ATOM 11795 61.873 OE1 GLN 749 57.664 1.00 29.51 B 0 ATOM 11796 NE2 GLN 87.443 63.116 1.00 27.64 749 56.039 В N 84. 984 84. 749 ATOM 11797 57.999 1.00 14.70 C GLN 749 54.348 B C ATOM 11798 GLN 57.015 1.00 14.10 0 749 55.054 В 0 ATOM 11799 HIS 84.147 58.440 1.00 13.44 N 750 53.415 В N 82.865 11800 CA HIS 57.808 53.174 1.00 12.63 ATOM 750 B C 82. 021 11801 HIS C ATOM CB 750 58.685 52.247 1.00 13.59 В 11802 80.587 ATOM CG HIS 750 58. 272 52.176 1.00 12.41 B C 11803 79.475 ATOM CD2 HIS 750 58.823 52.713 1.00 13.33 B C 11804 80.175 57.128 ATOM ND1 HIS 750 51.530 1.00 12.98 В N ATOM 11805 CE1 HIS 750 78.869 56.992 51.673 1.00 14.44 B C ATOM 11806 NE2 HIS 750 78.419 58.007 52.386 1.00 13.43 N ATOM 11807 C 82.985 52.595 1.00 13.84 HIS 750 56.404 В C

SUBSTITUTE SHEET (RULE 26)

53.011

1.00 14.53

В

0

82. 265 55. 499

ATOM

11808 0

HIS

750

				`						(Con	tinued)
					FI	G. 4-	242				
ATOM	11809	N	ILE	751	83.885		51.638	1.00 13.03	В	N	
ATOM	11810	CA	ILE	751	84.013		51.077	1.00 12.47	В	C	
ATOM ATOM	11811 11812	CB	ILE ILE	751 751	84. 927 86. 326	54. 838 55. 361	49. 814 50. 137	1.00 13.01 1.00 12.55	B B	C	
ATOM	11813		ILE	751	84. 999		49. 287	1.00 12.09	В	č	
ATOM	11814		ILE	751	85.677		47.939	1.00 11.16	B	С	
ATOM	11815	C	ILE	751	84.546		52.111	1.00 12.65	В	C	
ATOM	11816	0	ILE	751 750	84.025		52. 241	1.00 12.49	В	0	
ATOM ATOM	11817 11818	N CA	TYR TYR	752 752	85.575 86.137		52. 858 53. 850	1.00 13.74 1.00 14.04	B B	N C	
ATOM	11819	CB	TYR	752	87. 486		54.379	1.00 11.04	В	č	
ATOM	11820	CG	TYR	752	88. 628	53.468	53.472	1.00 9.86	В	С	
ATOM	11821		TYR	752	89.037		53.408	1.00 10.53	В	C	
ATOM	11822		TYR	752	90.015		52. 502	1.00 9.48	В	C	
ATOM ATOM	11823 11824		TYR TYR	752 752	89. 235 90. 219		52.608 51.692	1.00 9.66 1.00 8.36	B B	C	
ATOM	11825	CZ	TYR	752	90. 597	52.639	51.646	1.00 0.00	В	č	
ATOM	11826	ОH	TYR	752	91.536	52. 223	50.739	1.00 10.79	В	0	
ATOM	11827	C	TYR	752	85. 170		54. 973	1.00 13.42	В	C	
ATOM	11828	0	TYR	752	85. 176		55. 524	1.00 13.56	В	0	
ATOM ATOM	11829 11830	N Ca	THR THR	753 753	84. 323 83. 316		55. 295 56. 330	1.00 14.48 1.00 14.27	B B	N C	
ATOM	11831	CB	THR	753	82. 582		56.618	1.00 13.68	В	Č	
ATOM	11832	0G1	THR	753	83.519	56.136	57.130	1.00 17.48	B	0	
ATOM	11833	CG2		753	81.459	54.987	57.629	1.00 7.20	В	C	
ATOM	11834	C	THR	753	82.301	52. 849	55.815	1.00 16.15	В	C	
ATOM ATOM	11835 11836	O N	THR HIS	753 754	81.958 81.830	51. 894 53. 056	56. 508 54. 589	1.00 18.93 1.00 15.38	. B B	0 N	
ATOM	11837	CA	HIS	754	80. 840		53.999	1.00 16.06	В	Č	
ATOM	11838	CB	HIS	754	80. 424	52.666	52.620	1.00 15.26	В	C	
ATOM	11839	CG	HIS	754	79. 109		52. 162	1.00 16.39	В	C	
ATOM ATOM	11840		HIS	754	78. 779		51.095	1.00 15.75	В	C	
ATOM	11841 11842		HIS HIS	754 754	77. 936 76. 940	52.353 51.750	52.850 52.228	1.00 17.30 1.00 15.86	B B	N C	
ATOM	11843		HIS	754	77. 425	51.141	51.161	1.00 17.13	В	N	
ATOM	11844	C	HIS	754	81.349	50.731	53.886	1.00 16.28	B	C	
ATOM	11845	0	HIS	754	80. 639	49. 788	54. 238	1.00 17.31	В	0	
ATOM	11846 11847	N	MET	755 755	82.571	50. 564	53. 383	1.00 15.98	В	N	
ATOM ATOM	11848	CA CB	MET MET	755 755	83. 158 84. 532	49. 234 49. 300	53. 250 52. 573	1.00 16.05 1.00 15.41	B B	C	
ATOM	11849	CG	MET	755	84. 491	49.542	51.081	1.00 17.11	В	Č	
ATOM	11850	SD	MET	755	86.112	49.308	50.322	1.00 18.41	В	S	
ATOM	11851	CE	MET	755	86. 882	50.855	50. 742	1.00 20.74	В	С	
MOTA	11852	C	MET	755 756	83. 309	48. 582	54.623	1.00 15.38	В	C	
ATOM ATOM	11853 11854	O N	MET SER	755 756	83. 080 83. 701	47. 390 49. 371	54. 783 55. 614	1.00 13.30 1.00 15.36	B B	0 N	
ATOM	11855	CA	SER	756	83. 854	48. 833	56. 946	1.00 18.52	В	C	
ATOM	11856	CB	SER	756	84. 413	49.903	57.878	1.00 18.88	В	Č	
ATOM	11857	0G	SER	756	85. 723	50. 257	57. 477	1.00 18.74	В	0	

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(Continued) FIG. 4-243 C 1.00 19.14 48.282 57.462 SER 756 82.515 11858 C ATOM 57.975 1.00 19.94 0 В 82.464 47.158 SER 756 ATOM 11859 0 N 57.324 1.00 17.68 В 81.435 49.048 11860 HIS 757 ATOM N C 48.549 57.770 1.00 19.20 В 11861 HIS 757 80.134 CA ATOM C В 78.990 49.486 57.371 1.00 18.83 HIS 757 11862 CB ATOM C В 58.095 1.00 21.13 78.983 50.794 757 11863 CG HIS ATOM C 57.666 1.00 22.10 В 78.697 52.046 757 11864 CD2 HIS ATOM 79. 230 1.00 22.62 В N 50.899 59.447 ND1 HIS 757 **ATOM** 11865 1.00 23.60 79.096 59.820 B C 52.159 757 11866 HIS **ATOM** CE1 58.758 1.00 24.81 В N 78.772 52.876 757 11867 HIS **ATOM** NE2 57.120 1.00 17.94 В С 47.190 757 79.866 11868 HIS **ATOM** C B 0 1.00 16.58 57.772 HIS 757 79.416 46.251 **ATOM** 11869 0 В Ņ 80.158 55.828 1.00 17.93 47.103 PHE 758 **ATOM** 11870 N 79. 926 80. 286 В 45.888 55.052 1.00 18.80 PHE 758 **ATOM** 11871 CA B 46.138 53.586 1.00 15.70 CCCCCCATOM ATOM 11872 CB PHE 758 1.00 10.77 В 11873 52.677 CG 758 79.952 44.997 PHE В 52.251 1.00 8.39 CD1 PHE 78.646 44.790 11874 758 **ATOM** В 80.941 44.120 52.254 1.00 6.53 758 ATOM 11875 CD2 PHE 43.716 51.409 9.32 В 11876 758 78.334 1.00 **ATOM** CE1 PHE В 6.01 11877 CE2 PHE 758 80.638 43.045 51.417 1.00 ATOM В 42.836 50.991 2.78 758 79.340 1.00 **ATOM** 11878 CZ PHE C 80.697 44.674 55.560 1.00 20.68 В 11879 C PHE 758 **ATOM** 1.00 21.00 В 0 11880 0 PHE 758 80.110 43.631 55.851 ATOM В N 11881 N 759 82.014 44.811 55.654 1.00 23.57 ATOM ILE 1.00 25.05 В C 11882 759 82.858 43.722 56.117 **ATOM** CA ILE В $\begin{array}{c} C \\ C \\ C \end{array}$ ATOM 11883 CB ILE 759 84.364 44.129 56.069 1.00 25.44 B ATOM 11884 CG2 ILE 759 84.994 44.041 57.437 1.00 28.98 : 43.189 1.00 26.52 B ATOM 11885 CG1 ILE 759 85.128 55.142 43. 263 43. 318 84.706 53.704 1.00 26.84 B 759 ATOM 11886 CD1 ILE C 57.529 1.00 25.34 В 11887 759 82.441 ATOM C ILE 0 В 1.00 25.50 11888 0 ILE 759 82.420 42.136 57.866 ATOM 82.081 44.299 58.346 В N N 1.00 26.11 ATOM 11889 LYS 760 В 81.671 44.012 59.713 CCC 760 1.00 26.62 **ATOM** 11890 CA LYS B 1.00 26.43 LYS 760 81.444 45.300 60.487 ATOM 11891 CB B ATOM 11892 CG 760 82.178 45.298 61.792 1.00 29.00 LYS 45.271 В C 760 83.666 61.537 1.00 28.96 CD LYS ATOM 11893 61.250 1.00 30.01 C N 84.139 46.665 В 11894 LYS 760 **ATOM** CE 83.776 47.523 62.420 1.00 31.29 B 11895 LYS 760 ATOM NZ 80.406 43.179 59.740 1.00 27.08 В C 11896 **ATOM** LYS 760 80.312 42.200 60.473 В 0 1.00 28.46 **ATOM** 11897 LYS 760 11898 **GLN** 761 79.431 43.581 58.940 1.00 28.08 В N **ATOM** N 78.170 58.844 В C 11899 GLN 761 42.866 1.00 29.69 **ATOM** CA 77.213 43.652 57.942 1.00 31.26 B CCC **ATOM** 11900 CB GLN 761 76.072 42.855 57.347 1.00 34.99 B 11901 CG GLN 761 ATOM 76.477 56.072 1.00 37.85 B **GLN** 42.140 11902 CD 761 ATOM 55.062 1.00 37.29 B 0 76.800 42.775 0E1 GLN 761 ATOM 11903 56.112 1.00 39.80 B N NE2 GLN 761 76.464 40.808 ATOM 11904 58. 295 1.00 30.00 В C C GLN 761 78.401 41.456 11905 ATOM

77. 791

761

0

11906

ATOM

GLN

40.494

SUBSTITUTE SHEET (RULE 26)

58.753

1.00 31.14

В

0

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					FIG. 4-244	(Continued)
			0110	5 00		N
ATOM	11907	N	CYS	762	D 00 00 00	C
ATOM	11908	CA	CYS .	762	10.000	č
ATOM	11909	C	CYS	762	80. 275 39. 077 57. 712 1. 00 30. 21 B 80. 153 37. 860 57. 578 1. 00 29. 67 B	ŏ
ATOM	11910	0 CB	CYS CYS	· 762 762	80. 458 40. 212 55. 474 1. 00 30. 01 B	č
ATOM	11911 11912	CB SG	CYS	762	81. 198 38. 665 54. 849 1. 00 33. 72 B	Š
ATOM ATOM	11912	N	PHE	763	80. 986 39. 618 58. 698 1. 00 30. 53 B	Ň
ATOM	11913	CA	PHE	763	81.694 38.783 59.664 1.00 31.28 B	C
ATOM	11915	CB	PHE	763	83. 112 39. 310 59. 885 1. 00 29. 29 B	C
ATOM	11916		PHE	763	84. 052 39. 057 58. 736 1. 00 27. 21 B	C
ATOM	11917	CD1		763	83. 663 38. 280 57. 650 1. 00 26. 19 B	C
ATOM	11918		PHE	763	85. 348 39. 572 58. 762 1. 00 26. 38 B	C
ATOM	11919		PHE	763	84. 552 38. 015 56. 605 1. 00 27. 91 B	C
ATOM	11920	CE2	PHE	763	86. 249 39. 316 57. 727 1. 00 27. 36 B	C
ATOM	11921	CZ	PHE	763	85. 851 38. 533 56. 643 1. 00 27. 55 B	C
ATOM	11922	C	PHE	763	80. 994 38. 666 61. 011 1. 00 34. 52 B	
ATOM	11923	0	PHE	763	81. 473 37. 970 61. 908 1. 00 32. 78 B	0 N
ATOM	11924	N	SER	764	79. 862 39. 346 61. 151 1. 00 39. 49 B	N C
ATOM	11925	CA	SER	764	79. 099 39. 319 62. 393 1. 00 43. 60 B	C C
ATOM	11926	CB	SER	764	77. 860 40.199 62.273 1.00 44.56 B 78.218 41.528 61.948 1.00 50.05 B	0
ATOM	11927	OG	SER	764		C
ATOM	11928	C	SER	764 764	78. 668 37. 909 62. 746 1. 00 45. 96 B 77. 885 37. 289 62. 028 1. 00 45. 86 B	Ö
ATOM	11929 11930	O N	SER LEU	765	79. 189 37. 404 63. 856 1. 00 49. 22 B	Ň
ATOM ATOM	11931	CA	LEU	765	78. 845 36. 070 64. 317 1. 00 52. 03 B	Ċ
ATOM	11932	CB	LEU	765	79. 754 35. 678 65. 481 1. 00 52. 53 B	Č
ATOM	11933	CG	LEU	765	81. 234 35. 558 65. 115 1. 00 52. 85 B	Č
ATOM	11934		LEU	765	82.074 35.452 66.376 1.00 53.55 B	C
ATOM	11935		LEU	765	81. 435 34. 344 64. 214 1. 00 52. 54 B	С
ATOM	11936	C	LEU	765	77. 383 36. 069 64. 761 1. 00 54. 34 B	
ATOM	11937	0	LEU	765	77. 019 36. 721 65. 743 1. 00 53. 63 B	
ATOM	11938	N	PRO	766	76. 523 35. 340 64. 031 1. 00 56. 38 B	
ATOM	11939	CD	PRO	766	76. 833 34. 541 62. 831 1. 00 56. 67 B	
ATOM	11940	CA	PRO	766	75. 095 35. 263 64. 356 1. 00 57. 95 B	
ATOM	11941	CB	PRO	766	74. 509 34. 544 63. 141 1. 00 58. 24 B	
	11942	CG		766	75. 626 33. 633 62. 728 1. 00 57. 40 B	
ATOM	11943	C	PRO	766	74. 805 34. 523 65. 664 1. 00 59. 30 B	
ATOM	11944	0	PRO	766	73. 791 33. 789 65. 711 1. 00 60. 29 B 75. 584 34. 704 66. 627 1. 00 59. 84 B	
ATOM	11945	OXI	PRO	766	75. 584 34. 704 66. 627 1. 00 59. 84 B	
TER	11946	C1	PRO	766 901		
ATOM	11947	C1	NAG NAG	901	25.105 38.477 14.927 1.00 45.03 E 26.266 38.501 13.922 1.00 45.16 E	
ATOM	11948 11949	C2 N2	NAG	901	27. 447 39. 002 14. 595 1. 00 44. 20 E	
ATOM ATOM	11949	C7	NAG	901	28. 662 38. 702 14. 153 1. 00 43. 63 E	
ATOM		07	NAG	901	29. 050 37. 546 13. 997 1. 00 44. 60 E	ŏ
ATOM		C8	NAG	901	29. 588 39. 864 13. 838 1. 00 43. 83 E	
ATOM	11953	C3	NAG	901	25. 942 39. 385 12. 713 1. 00 46. 38 E	č
ATOM			NAG	901	26. 953 39. 235 11. 728 1. 00 49. 49 E	
ATOM			NAG	901	24.591 38.987 12.124 1.00 47.76 E	
					OUDSTITUTE OUEST (DUB C 26)	

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						(Continued)
					FIG. 4-245	(Continueu)
					_	•
ATOM	11956	04	NAG	901	24. 256 39. 836 11. 036 1. 00 49. 01 E	0
ATOM	11957	C5	NAG	901	23. 545 39. 104 13. 219 1. 00 49. 11 E	C
ATOM	11958	05	NAG	901	23. 858 38. 173 14. 276 1. 00 47. 99 E 22. 143 38. 804 12. 731 1. 00 50. 99 E	0 C
ATOM	11959	C6	NAG	901		0
ATOM	11960	06	NAG	901 902	21. 706 39. 781 11. 793 1. 00 53. 28 E 34. 526 67. 450 4. 248 1. 00 29. 71 E	Č
ATOM	11961	C1 C2	NAG NAG	902	33. 682 66. 990 3. 051 1. 00 31. 02 E	č
ATOM ATOM	11962 11963	N2	NAG	902	34. 077 65. 638 2. 692 1. 00 35. 02 E	Ň
ATOM	11964	C7	NAG	902	33. 181 64. 660 2. 610 1. 00 35. 78 E	Ċ
ATOM	11965	07	NAG	902	32. 213 64. 701 1. 852 1. 00 37. 59 E	Ō
ATOM	11966	C8	NAG	902	33.392 63.449 3.503 1.00 37.18 E	C
ATOM	11967	C3	NAG	902	33.927 67.915 1.848 1.00 31.67 E	C
ATOM	11968	03	NAG	902	33. 032 67. 583 0. 794 1. 00 34. 76 E	0
ATOM	11969	C4	NAG	902	33.753 69.386 2.248 1.00 31.76 E	C
ATOM	11970	04	NAG	902	34. 037 70. 238 1. 144 1. 00 30. 03 E	0
ATOM	11971	C5	NAG	902	34.701 69.674 3.412 1.00 30.64 E	C
ATOM	11972	05	NAG	902	34. 332 68. 844 4. 526 1. 00 30. 02 E	0
ATOM	11973	C6	NAG	902	34.720 71.114 3.892 1.00 30.81 E	C
ATOM	11974	06	NAG	902	33.457 71.512 4.409 1.00 34.26 E	0
ATOM	11975	CI	NAG	903	64. 239 77. 734 14. 341 1. 00 27. 20 E	C
ATOM	11976	C2	NAG	903	63.984 78.203 12.917 1.00 26.96 E	C
ATOM	11977	N2	NAG	903	63.551 77.080 12.116 1.00 25.19 E	N
ATOM	11978	C7	NAG	903	62.349 77.076 11.551 1.00 24.99 E	C
ATOM	11979	07	NAG	903	62.121 76.492 10.490 1.00 25.88 E	0
ATOM	11980	C8	NAG	903	61. 222 77. 800 12. 272 1. 00 23. 55 E	C C
ATOM	11981	C3	NAG	903	65. 253 78. 817 12. 325 1. 00 29. 00 E 64. 947 79. 400 11. 066 1. 00 29. 62 E	0
ATOM	11982	03	NAG	903		C
ATOM	11983	C4	NAG NAG	903 903	65. 814 79. 900 13. 248 1. 00 30. 83 E 67. 092 80. 316 12. 778 1. 00 31. 15 E	0
ATOM	11984 11985	04 C5	NAG	903	65.929 79.389 14.690 1.00 30.71 E	
ATOM ATOM	11986	05	NAG	903	64.669 78.842 15.133 1.00 30.11 E	
ATOM	11987	C6	NAG	903	66. 276 80. 502 15. 659 1. 00 32. 26 E	
ATOM	11988	06	NAG	903	65.937 80.144 16.993 1.00 35.52 E	
ATOM	11989	C1	NAG	904	56.857 73.229 -0.933 1.00 21.65 E	
ATOM	11990	C2	NAG	904	58. 289 73. 099 -1. 475 1. 00 21. 59 E	
ATOM	11991	N2	NAG	904	58.532 71.758 -1.961 1.00 21.40 E	
ATOM	11992	C7	NAG	904	58. 567 71. 523 -3. 267 1. 00 20. 76 E	
ATOM	11993	07	NAG	904	58.745 72.412 -4.104 1.00 18.55 E	
ATOM	11994	C8	NAG	904	58.371 70.080 -3.709 1.00 20.74 E	C
ATOM	11995	C3	NAG	904		C
ATOM	11996	03	NAG	904	60.611 73.413 -1.009 1.00 22.81 E	0
ATOM	11997	C4	NAG	904	59. 022 74. 832 0. 129 1. 00 22. 85 E	
ATOM	11998	04	NAG	904	59. 986 75. 217 1. 101 1. 00 24. 62 E	0
ATOM	11999	. C5	NAG	904	57. 634 74. 781 0. 737 1. 00 22. 86 E	
ATOM	12000	05	NAG	904	56.672 74.506 -0.297 1.00 21.95 E	
ATOM	12001	C6	NAG	904	57. 232 76. 083 1. 385 1. 00 24. 39 E	
ATOM	12002	06	NAG	904	57. 196 77. 133 0. 430 1. 00 31. 81 E	
ATOM	12003	C1	NAG	905	49.743 85.075 37.084 1.00 31.93 E	
ATOM	12004	C2	NAG	905	49.010 86.230 37.756 1.00 33.35 E	С

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					FIG. 4-246	(Continued)
						**
ATOM	12005	N2	NAG	905	47. 823 86. 586 37. 012 1. 00 34. 30 E	N C
ATOM	12006	C7	NAG	905	46. 648 86. 099 37. 395 1. 00 35. 18 E 46. 362 85. 888 38. 578 1. 00 36. 47 E	C 0
ATOM ATOM	12007 12008	07 C8	NAG NAG	905 905	46. 362 85. 888 38. 578 1. 00 36. 47 E 45. 640 85. 786 36. 303 1. 00 37. 15 E	C
ATOM	12008	C3	NAG	905	49.951 87.416 37.924 1.00 33.45 E	Č
ATOM	12010	03	NAG	905	49. 256 88. 512 38. 495 1. 00 33. 93 E	ŏ
ATOM	12011	C4	NAG	905	51. 043 86. 945 38. 863 1. 00 35. 37 E	č
ATOM	12012	04	NAG	905	51. 934 88. 009 39. 193 1. 00 35. 45 E	ŏ
ATOM	12013	Č5	NAG	905	51. 794 85. 773 38. 215 1. 00 34. 39 E	Č
ATOM	12014	05	NAG	905	50. 878 84. 684 37. 887 1. 00 32. 56 E	0
ATOM	12015	C6	NAG	905	52. 787 85. 212 39. 214 1. 00 36. 29 E	C
ATOM	12016	06	NAG	905	52.150 84.936 40.459 1.00 35.52 E	0
ATOM	12017	C1	NAG	906	128. 439 74. 792 56. 371 1. 00 36. 45 E	С
ATOM	12018	C2	NAG	906	127. 977 75. 856 55. 375 1. 00 37. 00 E	C
ATOM	12019	N2	NAG	906	126. 880 75. 335 54. 586 1. 00 37. 17 E	N
ATOM	12020	C7	NAG	906	125. 666 75. 871 54. 690 1. 00 38. 41 E	C
ATOM	12021	07	NAG	906	125. 264 76. 427 55. 714 1. 00 38. 52 E	0
ATOM	12022 12023	C8	NAG NAG	906 906	124.760 75.782 53.471 1.00 36.25 E 129.133 76.265 54.465 1.00 38.66 E	C
ATOM ATOM	12023	03	NAG	906	129.133 76.265 54.465 1.00 38.66 E 128.723 77.334 53.625 1.00 39.59 E	C 0
ATOM	12024	C4	NAG	906	130. 331 76. 704 55. 308 1. 00 39. 58 E	Ċ
ATOM	12026	04	NAG	906	131. 439 76. 975 54. 460 1. 00 41. 48 E	Ö
ATOM	12027	C5	NAG	906	130.699 75.602 56.312 1.00 40.24 E	Č
ATOM	12028	05	NAG	906	129. 556 75. 268 57. 133 1. 00 38. 27 E	ŏ
ATOM	12029	C6	NAG	906	131.811 76.032 57.255 1.00 41.89 E	Č
ATOM	12030	06	NAG	906	131. 906 75. 162 58. 378 1. 00 46. 70 E	0
ATOM	12031	C1	NAG	907	126.770 72.294 25.405 1.00 33.54 E	C
ATOM	12032	C2	NAG	907	127.763 73.454 25.478 1.00 35.73 E	C
ATOM	12033	N2	NAG	907	127. 401 74. 367 26. 540 1. 00 37. 97 E	Ņ
ATOM	12034	C7	NAG	907	128. 139 74. 400 27. 644 1. 00 41. 34 E	C
ATOM	12035	07	NAG	907	128. 715 73. 403 28. 094 1. 00 42. 96 E	0
ATOM	12036	C8	NAG	907	128. 278 75. 739 28. 352 1. 00 42. 60 E	C C
ATOM ATOM	12037 12038	C3 03	NAG NAG	907 907	127. 776 74. 167 24. 126 1. 00 36. 63 E 128. 692 75. 253 24. 154 1. 00 38. 28 E	0
ATOM	12039	C4	NAG	907	128. 171 73. 148 23. 047 1. 00 35. 89 E	C
ATOM	12040	04	NAG	907	128.191 73.758 21.763 1.00 35.85 E	0
ATOM	12041	C5	NAG	907	127. 161 71. 995 23. 075 1. 00 35. 12 E	Č
ATOM	12042	05	NAG	907	127.166 71.377 24.380 1.00 32.61 E	ŏ
ATOM	12043	C6	NAG	907	127. 444 70. 913 22. 057 1. 00 36. 17 E	č
ATOM	12044	06	NAG	907	128. 515 70. 083 22. 478 1. 00 38. 44 E	Ö
ATOM	12045	C1	NAG	908	97. 567 64. 129 12. 586 1. 00 33. 83 E	0 C C
ATOM	12046	C2	NAG	908	98. 226 65. 101 11. 602 1. 00 36. 51 E	С
ATOM	12047	N2	NAG	908	98. 466 66. 365 12. 269 1. 00 40. 33 E	N
ATOM	12048	C7	NAG	908	99. 645 66. 962 12. 148 1. 00 43. 03 E	С
ATOM	12049	07	NAG	908	100.703 66.434 12.500 1.00 45.77 E	0
ATOM	12050	C8	NAG	908	99. 655 68. 349 11. 529 1. 00 43. 86 E	C
ATOM	12051	C3	NAG	908	97. 328 65. 325 10. 380 1. 00 37. 11 E	C
ATOM	12052 12053	03 C4	NAG	908	98. 013 66. 122 9. 426 1. 00 37. 35 E	0
ATOM	14000	V4	NAG	908	96. 945 63. 975 9. 760 1. 00 36. 97 E	С

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					FIC	3. 4-	247			(Conti	nued)
ATOM	12054	04	NAG	908	96.049	64.165	8.668	1.00 36.08	E	0	
ATOM	12055	C5	NAG	908	96. 291	63.106	10.841	1.00 35.43	E	C	
ATOM	12056	05	NAG	908	97. 215	62.906	11.930	1.00 33.34	E	0	
ATOM	12057	C6	NAG	908	95.890	61.735	10.341	1.00 36.72	E	C	
ATOM	12058	06	NAG	908	95.085	61.057	11.296	1.00 38.75	E	0	
ATOM	12059	C1	NAG	909	106. 501	80.407	11.987	1.00 55.21	E	C	
ATOM	12060	C2	NAG	909	105.627	81.255	11.048	1.00 55.75	E	C	
ATOM	12061	N2	NAG	909	105. 631	82.658	11.427	1.00 55.80	E	N	
ATOM	12062	C7	NAG	909	106. 748	83. 259	11.828	1.00 56.83	E	C	
ATOM	12063	07	NAG	909	107. 685	83. 526	11.066	1.00 55.16	E	0	
ATOM	12064	C8	NAG	909	106. 838	83. 620	13. 305	1.00 56.25	E	C	
ATOM	12065	C3	NAG	909	104. 195	80. 724	11.087	1.00 56.36	E	C	
ATOM	12066	03	NAG	909	103. 396	81.452	10.166	1.00 58.58	E	0	
ATOM	12067	C4	NAG	909	104. 176	79. 229	10.744	1.00 56.19	E E	C 0	
ATOM	12068	04	NAG	909	102.855	78. 716 78. 478	10.862 11.692	1.00 55.29 1.00 56.24	E	C	
ATOM	12069	C5	NAG	909 909	105. 117 106. 446	79. 028	11.600	1.00 56.65	E.	0	
ATOM ATOM	12070 12071	05 C6	NAG NAG	909	105. 230	76. 996	11. 381	1.00 57.38	E	Č	
ATOM	12071	06	NAG	909	105. 230	76. 423	12.010	1.00 55.01	Ē	ŏ	
ATOM	12072	C1	NAG	910	105. 213	38. 428	20.006	1.00 34.33	Ë	Č	
ATOM	12074	C2	NAG	910	106. 113	37. 293	19. 498	1.00 37.27	Ē	č	
ATOM	12075	N2	NAG	910	107. 447	37. 789	19. 211	1.00 40.05	Ē	Ň	
ATOM	12076	C7	NAG	910	108. 495	36. 984	19.368	1.00 42.24	Ē	Ĉ	
ATOM	12077	07	NAG	910	109.013	36. 771	20. 465	1.00 42.65	E	0	
ATOM	12078	C8	NAG	910	109.047	36. 295	18. 126	1.00 42.65	E	C	
ATOM	12079	C3	NAG	910	105.504	36.650	18. 245	1.00 37.60	E	C	
ATOM	12080	03	NAG	910	106. 296	35. 547	17.831	1.00 38.44	E	0	
ATOM	12081	C4	NAG	910	104.084	36.182	18.551	1.00 36.63	E	C	
ATOM	12082	04	NAG	910	103. 489	35.616	17. 388	1.00 37.52	E	0	
ATOM	12083	C5	NAG	910	103. 274	37. 387	19.037	1.00 35.81	Ē	C	
ATOM	12084	05	NAG	910	103. 883	37. 930	20. 229	1.00 34.96	E	0	
ATOM	12085	C6	NAG	910	101.838	37. 042	19.385	1.00 34.79	E	C	
ATOM	12086	06	NAG	910	101. 781	36.089	20. 437	1.00 34.77	E	0	
TER	12087	^	NAG	910	FO 405	00 704	10 170	1 00 10 00	E	•	
ATOM	12088	0	HOH	1	53. 435	80. 704	18. 172	1.00 10.60	W	0	
ATOM	12089	0	HOH	2	57.473	78. 703	26. 320	1.00 21.03	W	0	
				3				1.00 7.09	W		
ATOM	12091 12092	0	HOH	4	56. 235 58. 127	76. 520	22. 816 28. 066	1.00 14.76 1.00 4.57	W	0	
ATOM ATOM	12092	.0	HOH HOH	5 6	40. 099	60. 758 59. 877	48. 410	1.00 4.37	W	0 0	
ATOM	12093	0	НОН	6 7	29. 796	47. 323	37. 410	1.00 24.76	W	0	
ATOM	12094	0	HOH	8	38. 634	67. 195	51.371	1.00 22.65	Ϋ́	0	
ATOM	12096	Ö	HOH	9	41.732	52. 103	37. 673	1.00 13.34	Ÿ	Ő	
ATOM	12097	0	HOH	10	79. 275	54. 159	21.409	1.00 15.53	Ÿ	Ö	
ATOM	12098	Ö	НОН	11	65. 287	66. 160	35. 128	1.00 7.29	Ÿ	Ŏ	
ATOM	12099	ŏ	НОН	12	79. 267	49. 364	26. 780	1.00 14.00	Ÿ	ŏ	
ATOM	12100	Ŏ	НОН	13	67. 989	56. 792	26. 833	1.00 20.21	Ÿ	ŏ	
ATOM	12101	Ö	НОН	14.	68. 995	70. 138	19.815	1.00 12.98	Ÿ	ŏ	
ATOM	12102	0	HOH	15	59. 193	63.441	21.787	1.00 5.68	W	0	

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										(Continued)
					FIG.	4 -	2 4 8			
ATOM	12103	0	НОН	16		66.700	47. 886	1.00 13.21	W	0
ATOM	12104	0	НОН	17		3.043	50.567	1.00 20.65	W	0
ATOM	12105	0	НОН	18		39.817	52.424	1.00 34.74	W	0
ATOM	12106	0	HOH	19		39.650	29.378	1.00 25.18	W	0
ATOM	12107	0	HOH	20		31. 115 35. 282	48. 431 28. 107	1.00 18.77 1.00 27.06	W	0 0
ATOM	12108 12109	0	HOH HOH	21 22		33. 930	21.686	1.00 27.00	W	0
ATOM ATOM	12110	0	HOH	23		37. 394	23. 730	1.00 23.10	W	ŏ
ATOM	12111	Ö	НОН	24		57. 109	30. 405	1.00 21.66	W	Ŏ
ATOM	12112	ŏ	НОН	25		30.303	31.025	1.00 34.33	W	Õ
ATOM	12113	0	HOH	26		66.634	22.568	1.00 10.18	W	0
ATOM	12114	0	HOH	27		54. 838	52.427	1.00 29.90	A	0
ATOM	12115	0	HOH	28		30.961	23. 145	1.00 17.51	W	0
ATOM	12116	0	НОН	29		71.484	27.824	1.00 34.92	M	0
ATOM	12117	0	HOH	30		57.060	34. 794	1.00 28.05	W	0
ATOM	12118	0	HOH	31		72.092	24. 987	1.00 14.46 1.00 22.75	W	0
ATOM ATOM	12119 12120	0	HOH HOH	32 33		84. 543 63. 840	25. 502 46. 551	1.00 22.75	W	0 .
ATOM	12121	0	НОН	34		17. 441	47. 587	1.00 25.33	Ÿ	0
ATOM	12122	ő	НОН	35		56.510	44. 904	1.00 30.51	Ÿ	ŏ
ATOM	12123	Ö	НОН	36	31.114	59. 222	42. 224	1.00 13.22	W	0
ATOM	12124	0	HOH	37		64. 199	47.510	1.00 21.69	W	0
ATOM	12125	0	HOH	38		70. 385	33.904	1.00 24.19	W	0
ATOM	12126	0	НОН	39		17.056	34. 998	1.00 24.19	W	0
ATOM	12127	0	НОН	40		49. 571	32. 910	1.00 22.85	W	0
ATOM	12128	0	HOH	41		53.516	39. 573	1.00 12.47	W	0
ATOM	12129	0	HOH	42		48. 248 53. 457	21.021	1.00 24.35 1.00 32.23	W	0
ATOM ATOM	12130 12131	0	HOH HOH	43 44		61.003	19. 457 21. 232	1.00 32.23	W	0 0
ATOM	12132	0.	НОН	45		50. 325	19.619	1.00 36.05	Ÿ	Ö
ATOM	12133	0	НОН	46		58. 001	59.062	1.00 20.53	Ÿ	ŏ
MOTA	12134	Ŏ	НОН	47		54. 978	15. 598	1.00 20.74	Ÿ	Ŏ
ATOM	12135	Ŏ	НОН	48		51.103	23.882	1.00 16.65	W	0
ATOM	12136	0	HOH	49	31.428	66. 281	21.097	1.00 18.82	W	0
ATOM	12137	0	HOH	50 ·		72. 589	-9.525	1.00 19.51	W	0
ATOM	12138	0	НОН	51		47. 337	39. 374	1.00 16.49	Ŋ	0
ATOM	12139	0	HOH	52 50		68.673	61. 331	1.00 26.41	W	0
ATOM	12140	0	HOH	53		48. 947	47.621	1.00 17.49	W	0
ATOM	12141	0	HOH HOH	54 55		82. 021 45. 427	10. 956 40. 043	1.00 24.56 1.00 35.52	W W	0
ATOM ATOM	12142 12143	0	НОН	55 56		60. 491	43. 209	1.00 33.32	W	0
ATOM	12143	0	НОН	57		62.843	34. 752	1.00 10.13	Ÿ	0
ATOM	12145	ŏ	НОН	58		55.643	2. 123	1.00 19.51	Ÿ	ŏ
ATOM	12146	ŏ	НОН	59		45. 985	50.017	1.00 22.18	Ÿ	Ö ·
ATOM	12147	Ö	НОН	60		70. 566	0.317	1.00 32.17	Ÿ	Ö
ATOM	12148	0	HOH	61	61.782	69. 597	25.094	1.00 13.27	W	0
ATOM	12149	0	НОН	62		79. 521	14.538	1.00 17.25	W	0
ATOM	12150	0	HOH	63		86.907	16. 122	1.00 21.54	Ŋ	0
ATOM	12151	0	НОН	64	49. 536	54. 337	14. 938	1.00 22.27	₩	0

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					FIG	. 4 -	250			(Continued)
ATOM ATOM	12201 12202	0	НОН НОН	114 115	41.491 64.362	58. 601 64. 567	0. 047 16. 259	1.00 42.91 1.00 24.97	₩	0 0
ATOM	12203	ŏ	НОН	116	43. 928	76. 242	2. 332	1.00 21.69	Ÿ	Ö
ATOM	12204	0	HOH	117	80. 703	69.349	43.827	1.00 28.64	W	0
ATOM	12205	0	HOH	118	81.671	48. 368	20. 456	1.00 15.16	W	0
ATOM	12206	0	HOH	119		71.127	54.004 47.288	1.00 22.01	W	0
ATOM ATOM	12207 12208	0	НОН НОН	120 121	27. 474 69. 871	69. 426 60. 279	33. 380	1.00 26.74 1.00 13.47	W W	0 0
ATOM	12200	0	НОН	122	67. 879	38. 425	47. 297	1.00 25.68	"	0
ATOM	12210	ő	НОН	123	41.866	62. 152	36. 306	1.00 27.91	Ÿ	Ŏ
ATOM	12211	ŏ	НОН	124	82. 055	50. 923	20. 718	1.00 23.09	Ÿ	Ö
ATOM	12212	0	НОН	125	38. 821	82.651	33.998	1.00 14.04	W	0
ATOM	12213	0	HOH	126	64. 420	42.195	31.710	1.00 28.88	W	0
ATOM	12214	0	НОН	127	60.713	36. 262	43.885	1.00 22.95	W	0
ATOM	12215	0	HOH	128	63. 095	38. 041	44.744	1.00 26.42	W	0
ATOM	12216	0	HOH	129	36.718	65. 633	50.633	1.00 38.12	W	0
ATOM	12217	0	HOH HOH	130	55. 575 41. 981	80.086	20. 196 15. 577	1.00 26.23 1.00 23.62	W W	0 .
ATOM ATOM	12218 12219	0	НОН	131 132	41. 961	65. 129 75. 632	53. 563	1.00 25.02	W	0 0
ATOM	12220	Ö	НОН	133	75. 617	59. 792	32.116	1.00 35.58	W	0
ATOM	12221	ŏ	НОН	134	73. 522	67. 486	30. 484	1.00 21.07	W	ŏ
ATOM	12222	Ŏ	НОН	135		81.671	30.091	1.00 41.74	W	Ö
ATOM	12223	0	HOH	136	41.663	53.300	13.574	1.00 39.95	W	0
ATOM	12224	0	HOH	137	42.885	39.029	29.960	1.00 29.57	W	0
ATOM	12225	0	НОН	138		56.683	24. 253	1.00 37.19	W	0
ATOM	12226	0	НОН	139		54. 591	37. 133	1.00 19.60	W	0
ATOM	12227	0	HOH	140		48. 505	51.547	1.00 22.87	W	. 0
ATOM ATOM	12228 12229	0	НОН НОН	141 142	105. 346 108. 946	35. 319 33. 058	45. 478 43. 850	1.00 6.28 1.00 17.18	. ₩	0
ATOM	12230	0	HOH	143	100. 340	50. 291	32. 321	1.00 17.18	. n W	0 0
ATOM	12231	ő	НОН	144		56. 732	33. 886	1.00 12.23	Ψ̈́	0
ATOM	12232	ŏ	НОН	145	96. 721	59. 108	34. 335	1.00 14.59	Ÿ	ŏ
ATOM	12233	Ŏ	НОН	146		66.436	57.099	1.00 19.53	Ÿ	Ö
ATOM	12234	0	HOH	147	107. 303	38.674	48.678	1.00 12.12	W	0
ATOM	12235	0	HOH	148		54.174	15.770	1.00 18.02	W	0
ATOM	12236	0	HOH	149				1.00 13.93	W	0
ATOM	12237	0	HOH	150		67. 497	30. 740	1.00 26.00	W	0
ATOM	12238	0	НОН	151		54. 147	45.005	1.00 10.46	W	0
ATOM ATOM	12239 12240	0	HOH HOH	152 153		55. 650 55. 414	9. 401 40. 305	1.00 27.03 1.00 14.32	₩ W	0
ATOM	12240	0	HOH	154		40. 670	45. 200	1.00 14.32	n W	0 0
ATOM	12242	ŏ	НОН	155		37. 761	27. 531	1.00 10.00	Ψ̈́	0
ATOM	12243	ŏ		156		62.914	36.962	1.00 26.29	w	0
ATOM	12244	Ŏ	НОН	157		65. 229	44.012	1.00 37.02	Ÿ	ŏ
ATOM	12245	0	HOH	158		46. 435	54.377	1.00 26.11	Ÿ	Ŏ
ATOM	12246	0	НОН	159		40.104	43.504	1.00 11.71	14	0
ATOM	12247	0	НОН	160		42. 243	44.636	1.00 14.84	W	0
ATOM	12248	0	HOH	161		56.669	35.498	1.00 35.54	M	0
ATOM	12249	0	НОН	162	88. 481	51.896	31.163	1.00 12.64	W	0

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									(Continued)
					FIG. 4-2	251			•
ATOM	12250	0	НОН	163	95. 169 58. 602	25. 005	1.00 10.78	W	0
ATOM	12251	0	HOH	164	115. 235 34. 630	45. 444	1.00 26.24	W	0
ATOM	12252	0	HOH	165		55. 571	1.00 20.62	W	0
ATOM	12253	0	HOH	166		19.482	1.00 36.24	W	0
ATOM	12254	0	HOH	167		46. 942	1.00 20.56	W	0
ATOM	12255	0	HOH	168		37. 270	1.00 21.34	Ä	0
ATOM	12256	0	HOH	169		31.569	1.00 23.37 1.00 18.43	W	0
ATOM ATOM	12257 12258	0	H0H H0H	170 171		48. 086 32. 584	1.00 18.43	MA M	0 0
ATOM	12259	0	ноп НОН	172		28. 628	1.00 22.93	Ÿ	0
ATOM	12260	0	HOH	173		56.950	1.00 25.07	Ÿ	0
ATOM	12261	0	НОН	174		11.178	1.00 23.37	Ÿ	Ö
ATOM	12262	ŏ	НОН	175		51.786	1.00 19.27	Ÿ	ŏ
ATOM	12263	Õ	НОН	176		55.683	1.00 19.54	W	Ö
ATOM	12264	0	НОН	177		44.832	1.00 25.55	W	0
ATOM	12265	0	HOH	178		27. 707	1.00 29.36	W	0
ATOM	12266	0	HOH	179		23.388	1.00 28.01	W	0
ATOM	12267	0	HOH	180		50. 278	1.00 16.30	W	0
ATOM	12268	0	HOH	181		29. 465	1.00 7.47	W	0
ATOM	12269	0	HOH	182		29. 409	1.00 28.14	W	0
ATOM	12270	0	HOH	183		45. 877	1.00 22.55	Ŋ	0
ATOM	12271	0	HOH	184		44.078	1.00 28.83	W	0
ATOM ATOM	12272 12273	0 0	HOH ·	185 186		29. 778	1.00 31.97	W	0
ATOM	12274	0	HOH	187		34. 566 40. 032	1.00 18.77 1.00 18.28	W	0 0
ATOM	12275	Ö	НОН	188		36. 341	1.00 18.28	W	0
ATOM	12276	Ö	НОН	189		33. 025	1.00 20.03	W	0
ATOM	12277	Ŏ	НОН	190		15. 989	1.00 34.45	Ÿ	ŏ
ATOM	12278	Ŏ	НОН	191		35.865	1.00 10.27	Ÿ	ŏ
ATOM	12279	0	HOH	192		57. 881	1.00 13.62	W	Ö
ATOM	12280	0	HOH	193		32. 830	1.00 19.19	W	0
ATOM	12281	0	НОН	194		38. 393	1.00 26.68	W	0
ATOM	12282	0	HOH	195		33. 937	1.00 24.15	W	0
ATOM	12283	0	НОН	196		31.652	1.00 12.71	W	0
ATOM	12284	0	НОН	197		54. 587	1.00 10.61	W	0
ATOM	12285	0	НОН	198	109.915 41.219 3	37.675	1.00 19.28	W	0
ATOM	12286	0	НОН	199		27. 926	1.00 9.03	W	0
ATOM ATOM	12287 12288	0	НОН НОН	200 201		34.046	1.00 8.20	W	0
ATOM	12289	0	НОН	201		3.124	1.00 15.97 1.00 22.83	W	0
ATOM	12290	0	НОН	202		3. 499 17. 689	1.00 22.83	¥	0 0
ATOM	12291	Ö	HOH	204		6.885	1.00 12.08	W	0
ATOM	12292	Ö	НОН	205		33. 261	1.00 15.83	Ÿ	0
ATOM	12293	Ö	НОН	206		6. 273	1.00 17.78	Ÿ	Ŏ
ATOM	12294	Ö	HOH	207		5. 944	1.00 23.96	Ÿ	Ŏ
ATOM	12295	0	HOH	208		4. 587	1.00 12.16	Ÿ	Ö
ATOM	12296	0	HOH	209	114. 209 49. 450 3	86.803	1.00 19.70	W	0
ATOM	12297	0	НОН	210		9. 990	1.00 33.63	W	0
ATOM	12298	0	НОН	211	95.004 41.032 1	4. 678	1.00 29.66	W	0

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ATOM 12299 0 HOH 212 113.170 36.816 43.347 1.00 21.90 W 0 ATOM 12300 0 HOH 213 77.770 71.277 45.572 1.00 31.73 W 0 ATOM 12301 0 HOH 214 128.636 66.746 61.783 1.00 37.87 W 0 ATOM 12302 0 HOH 215 128.566 42.261 18.644 1.00 26.655 W 0 ATOM 12303 0 HOH 216 135.349 43.830 34.280 1.00 24.699 W 0 ATOM 12304 0 HOH 217 85.640 67.686 27.706 1.00 32.33 W 0 ATOM 12305 0 HOH 218 93.669 46.427 45.5066 1.00 24.89 W 0 ATOM 12306 0 HOH 219 17.799 67.819 59.317 1.00 20.28 W 0 ATOM 12307 0 HOH 220 79.954 55.009 6.2399 1.00 19.13 W 0 ATOM 12308 0 HOH 221 17.228 62.083 29.483 1.00 25.50 W 0 ATOM 12308 0 HOH 221 17.228 62.083 29.483 1.00 25.50 W 0 ATOM 12301 0 HOH 222 105.505 51.938 31.912 1.00 35.19 W 0 ATOM 12310 0 HOH 222 107.489 60.380 64.395 1.00 24.39 W 0 ATOM 12310 HOH 223 166.835 57.215 14.677 1.00 21.77 W 0 ATOM 12310 HOH 224 107.489 60.380 64.395 1.00 24.39 W 0 ATOM 12310 HOH 224 107.489 60.380 64.395 1.00 24.39 W 0 ATOM 12310 HOH 224 107.489 60.380 64.395 1.00 24.39 W 0 ATOM 12310 HOH 224 107.489 60.380 64.395 1.00 24.39 W 0 ATOM 12310 HOH 224 107.489 60.380 64.395 1.00 24.39 W 0 ATOM 12310 HOH 225 79.753 74.355 77.299 1.00 35.59 W 0 ATOM 12310 HOH 226 116.807 64.679 29.466 1.00 24.83 W 0 ATOM 12310 HOH 226 106.295 62.225 36.826 1.00 26.06 W 0 ATOM 12310 HOH 227 87.239 82.355 64.706 1.00 21.19 W 0 ATOM 12310 HOH 228 1.916 67.98 41.81 1.00 16.54 W 0 ATOM 12310 HOH 233 93.378 45.857 52.934 1.00 12.19 W 0 ATOM 12310 HOH 233 93.378 45.857 52.934 1.00 12.19 W 0 ATOM 12320 HOH 233 93.378 45.857 52.934 1.00 12.19 W 0 ATOM 12323 HOH 234 132.099 46.877 33.399 1.00 1.00 2.97 W 0 ATOM 12323 HOH 235 93.378 45.857 52.934 1.00 12.10 W 0 ATOM 12330 HOH 236 93.289 66.822 37.895 1.00 26.19 W 0 ATOM 12331 HOH 237 93.716 62.21 12.5521 1.00 13.10 W 0 ATOM 12323 HOH 236 93.249 60.882 37.895 1.00 26.19 W 0 ATOM 12333 HOH 244 195.657 65.858 15.602 1.00 19.17 W 0 ATOM 12334 HOH 247 14.489 60.385 63.99 1.00 13.21 W 0 ATOM 12333 HOH 244 95.57 1.768 84.89 33.99 1.00 10.17 W 0 ATOM 12334 HOH 247 14.489 60.38 60.38 1.00 18.40 W 0 ATOM 12334 HOH 248 1											(Continued)
ATOM 12309 0 HOH 212 113.170 36.816 43.347 1.00 21.90 W 0 ATOM 12301 0 HOH 213 77.770 71.277 45.572 1.00 31.73 W 0 ATOM 12302 0 HOH 215 128.566 42.766 61.783 1.00 37.87 W 0 ATOM 12303 0 HOH 215 128.566 42.766 118.644 1.00 26.55 W 0 ATOM 12303 0 HOH 216 135.349 43.830 34.280 1.00 24.69 W 0 ATOM 12304 0 HOH 217 85.640 67.686 27.705 1.00 32.33 W 0 ATOM 12305 0 HOH 218 93.669 46.427 45.506 1.00 24.39 W 0 ATOM 12306 0 HOH 219 117.990 67.819 59.317 1.00 20.28 W 0 ATOM 12307 0 HOH 221 17.990 67.819 59.317 1.00 20.28 W 0 ATOM 12308 0 HOH 221 17.288 62.083 29.483 1.00 29.50 W 0 ATOM 12309 0 HOH 222 165.505 51.983 81.912 1.00 35.13 W 0 ATOM 12310 0 HOH 223 106.835 57.215 14.677 1.00 21.77 W 0 ATOM 12310 0 HOH 224 107.489 60.380 64.395 1.00 24.83 W 0 ATOM 12311 0 HOH 225 17.753 74.355 53.7799 1.00 35.35 W 0 ATOM 12313 0 HOH 222 106.835 57.215 14.677 1.00 21.77 W 0 ATOM 12313 0 HOH 225 16.807 64.679 29.466 1.00 24.83 W 0 ATOM 12313 0 HOH 227 87.239 52.355 64.706 1.00 24.83 W 0 ATOM 12315 0 HOH 227 87.239 52.355 64.706 1.00 24.83 W 0 ATOM 12316 0 HOH 228 81.916 67.988 41.878 1.00 14.54 W 0 ATOM 12317 0 HOH 227 87.299 52.355 64.706 1.00 21.83 W 0 ATOM 12318 0 HOH 227 87.299 52.355 64.706 1.00 21.83 W 0 ATOM 12318 0 HOH 227 87.399 52.355 64.706 1.00 21.90 W 0 ATOM 12318 0 HOH 232 80.95 62.226 80.826 1.00 26.06 W 0 ATOM 12318 0 HOH 233 80.925 62.248 53.3991 1.00 15.40 W 0 ATOM 12318 0 HOH 233 80.925 62.248 53.3991 1.00 15.00 W 0 ATOM 12320 0 HOH 233 80.925 62.248 53.3991 1.00 15.00 W 0 ATOM 12321 0 HOH 230 88.57 49.558 53.991 1.00 15.00 W 0 ATOM 12323 0 HOH 233 80.95 65.56 55.66 7.06 1.00 21.19 W 0 ATOM 12333 0 HOH 234 132.069 46.877 33.333 1.00 29.97 W 0 ATOM 12331 0 HOH 230 88.57 49.558 53.991 1.00 15.40 W 0 ATOM 12332 0 HOH 233 80.95 65.56 67.06 1.00 29.98 W 0 ATOM 12332 0 HOH 234 132.069 46.877 33.333 1.00 29.97 W 0 ATOM 12333 0 HOH 234 132.069 46.877 33.333 1.00 29.97 W 0 ATOM 12333 0 HOH 244 17.688 49.89 33.774 1.00 23.88 W 0 ATOM 12334 0 HOH 244 17.788 55.50 67.06 1.00 1.19 W 0 ATOM 12333 0 HOH 244 17.788 65.80 85.80 1.						· FIC	7. 4 -	252			(Continued)
ATOM 12301 0 HOH 213 77.770 71.277 45.572 1.00 31.73 W 0 ATOM 12302 0 HOH 214 128.636 66.746 61.783 1.00 37.87 W 0 ATOM 12303 0 HOH 215 128.566 42.261 18.644 1.00 26.65 W 0 ATOM 12303 0 HOH 216 155.349 43.830 34.280 1.00 24.69 W 0 ATOM 12304 0 HOH 217 85.640 67.686 27.706 1.00 32.33 W 0 ATOM 12305 0 HOH 218 93.669 46.427 45.506 1.00 22.33 W 0 ATOM 12306 0 HOH 219 117.990 67.819 59.317 1.00 24.39 W 0 ATOM 12307 0 HOH 220 79.954 55.099 62.309 1.00 19.13 W 0 ATOM 12308 0 HOH 221 117.228 62.083 29.483 1.00 29.50 W 0 ATOM 12309 0 HOH 221 117.228 62.083 29.483 1.00 29.50 W 0 ATOM 12310 0 HOH 222 105.505 51.938 31.912 1.00 35.19 W 0 ATOM 12310 0 HOH 222 105.505 51.938 31.912 1.00 35.19 W 0 ATOM 12311 0 HOH 224 107.489 60.380 64.395 1.00 24.53 W 0 ATOM 12313 0 HOH 225 116.807 64.679 29.466 1.00 21.77 W 0 ATOM 12313 0 HOH 226 116.807 64.679 29.466 1.00 21.17 W 0 ATOM 12313 0 HOH 227 87.235 52.355 64.706 1.00 24.83 W 0 ATOM 12314 0 HOH 227 87.235 52.355 64.706 1.00 24.83 W 0 ATOM 12315 0 HOH 228 81.916 67.988 41.878 1.00 14.54 W 0 ATOM 12316 0 HOH 230 78.057 49.535 53.991 1.00 14.54 W 0 ATOM 12318 0 HOH 231 99.787 47.673 22.572 1.00 18.00 W 0 ATOM 12318 0 HOH 231 99.787 47.673 22.572 1.00 18.00 W 0 ATOM 12318 0 HOH 231 99.787 47.673 22.572 1.00 18.00 W 0 ATOM 12319 0 HOH 233 93.916 62.211 25.521 1.00 13.10 W 0 ATOM 12320 0 HOH 233 93.916 62.211 25.521 1.00 13.10 W 0 ATOM 12320 0 HOH 234 132.099 46.877 33.393 1.00 20.97 W 0 ATOM 12320 0 HOH 234 132.099 46.877 33.393 1.00 20.97 W 0 ATOM 12320 0 HOH 234 132.099 46.877 33.393 1.00 20.97 W 0 ATOM 12320 0 HOH 234 132.099 46.877 33.393 1.00 20.97 W 0 ATOM 12320 0 HOH 234 132.099 46.877 33.393 1.00 20.97 W 0 ATOM 12320 0 HOH 234 132.099 46.877 33.393 1.00 20.97 W 0 ATOM 12320 0 HOH 234 132.099 46.877 33.393 1.00 20.97 W 0 ATOM 12320 0 HOH 234 132.099 46.877 33.393 1.00 20.97 W 0 ATOM 12332 0 HOH 244 19.55 87.56 87.56 87.59 1.00 13.10 W 0 ATOM 12332 0 HOH 247 17.688 49.899 1.00 13.21 W 0 ATOM 12333 0 HOH 247 17.688 49.899 1.00 13.21 W 0 ATOM 12334 0 HOH 247 17.688 49.899 1.00 13.								202			
ATOM 12301 0 HOH 213	ATOM	12299	0	НОН	212	113.170	36.816	43. 347	1.00 21.90	W	0
ATOM 12303 0 HOH 215 128.566 42.261 18.644 1.00 26.65					213	77.770				W	0
ATOM 12304 0 HOH 216 135.349 43.830 34.280 1.00 24.69 W 0 ATOM 12305 0 HOH 217 85.640 67.686 27.706 1.00 32.33 W 0 ATOM 12305 0 HOH 218 93.669 46.427 45.506 1.00 24.39 W 0 ATOM 12307 0 HOH 229 117.990 67.819 59.317 1.00 20.28 W 0 ATOM 12308 0 HOH 221 117.286 65.009 62.309 1.00 19.13 W 0 ATOM 12309 0 HOH 222 117.288 62.083 29.483 1.00 29.50 W 0 ATOM 12310 0 HOH 222 106.835 57.215 14.677 1.00 21.777 W 0 ATOM 12311 0 HOH 224 107.489 60.380 64.395 1.00 24.53 W 0 ATOM 12311 0 HOH 224 107.489 60.380 64.395 1.00 24.53 W 0 ATOM 12313 0 HOH 226 116.807 64.679 29.466 1.00 21.777 W 0 ATOM 12314 0 HOH 227 87.239 52.355 64.706 1.00 21.77 W 0 ATOM 12315 0 HOH 228 16.807 64.679 29.466 1.00 24.83 W 0 ATOM 12316 0 HOH 229 106.295 62.226 36.826 1.00 26.06 W 0 ATOM 12317 0 HOH 230 78.057 49.553 53.991 1.00 14.54 W 0 ATOM 12318 0 HOH 231 99.797 47.673 22.572 1.00 15.40 W 0 ATOM 12319 0 HOH 232 80.925 62.495 87.326 1.00 24.08 W 0 ATOM 12320 0 HOH 234 132.069 46.877 33.339 1.00 20.97 W 0 ATOM 12320 0 HOH 235 93.378 45.857 57.251 1.00 15.40 W 0 ATOM 12320 0 HOH 234 132.069 46.877 33.339 1.00 20.97 W 0 ATOM 12320 0 HOH 235 93.378 45.857 55.10 1.00 15.40 W 0 ATOM 12320 0 HOH 235 93.378 45.857 55.10 1.00 15.40 W 0 ATOM 12320 0 HOH 235 93.378 45.857 55.10 1.00 15.40 W 0 ATOM 12320 0 HOH 236 93.249 60.882 37.895 1.00 20.97 W 0 ATOM 12320 0 HOH 236 93.249 60.882 37.895 1.00 20.97 W 0 ATOM 12320 0 HOH 236 93.249 60.882 37.895 1.00 20.97 W 0 ATOM 12320 0 HOH 240 87.009 55.227 64.894 1.00 13.10 W 0 ATOM 12320 0 HOH 242 117.688 49.829 33.274 1.00 13.10 W 0 ATOM 12330 0 HOH 242 117.688 49.829 33.274 1.00 13.21 W 0 ATOM 12330 0 HOH 242 117.688 49.829 33.274 1.00 13.21 W 0 ATOM 12330 0 HOH 242 117.688 49.829 33.578 1.00 22.69 W 0 ATOM 12330 0 HOH 242 117.688 49.829 35.579 1.00 28.88 W 0 ATOM 12330 0 HOH 245 100.413 48.087 60.147 1.00 23.84 W 0 ATOM 12330 0 HOH 247 124.287 57.266 34.284 1.00 15.90 W 0 ATOM 12330 0 HOH 247 124.287 57.266 34.284 1.00 15.90 W 0 ATOM 12333 0 HOH 245 100.413 48.087 60.147 1.00 23.80 W 0 ATOM 123340 0 HOH 257 117.356 56	ATOM	12301	0	HOH							
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ATOM 12330											
ATOM 12331											
ATOM 12332											
ATOM 12333											
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ATOM 12335											
ATOM 12336			-								
ATOM 12337											
ATOM 12338 0 HOH 251 101.409 54.086 55.370 1.00 24.76 W 0 ATOM 12339 0 HOH 252 116.022 62.795 46.555 1.00 17.19 W 0 ATOM 12340 0 HOH 253 95.637 65.687 28.739 1.00 22.07 W 0 ATOM 12341 0 HOH 254 89.440 32.347 36.665 1.00 21.89 W 0 ATOM 12342 0 HOH 255 86.628 29.295 53.611 1.00 28.08 W 0 ATOM 12343 0 HOH 256 102.111 48.926 69.771 1.00 28.02 W 0 ATOM 12344 0 HOH 257 117.835 65.790 61.089 1.00 30.23 W 0 ATOM 12345 0 HOH 258 105.286 61.859 63.757 1.00 33.92 W 0 ATOM 12346 0 HOH 259 86.743 64.218 34.930 1.00 28.91 W 0 ATOM 12347 0 HOH 260 105.249 47.160 40.635 1.00 20.28 W 0											
ATOM 12339			0								
ATOM 12340 0 HOH 253 95.637 65.687 28.739 1.00 22.07 W 0 ATOM 12341 0 HOH 254 89.440 32.347 36.665 1.00 21.89 W 0 ATOM 12342 0 HOH 255 86.628 29.295 53.611 1.00 28.08 W 0 ATOM 12343 0 HOH 256 102.111 48.926 69.771 1.00 28.02 W 0 ATOM 12344 0 HOH 257 117.835 65.790 61.089 1.00 30.23 W 0 ATOM 12345 0 HOH 258 105.286 61.859 63.757 1.00 33.92 W 0 ATOM 12346 0 HOH 259 86.743 64.218 34.930 1.00 28.91 W 0 ATOM 12347 0 HOH 260 105.249 47.160 40.635 1.00 20.28 W 0			0	HOH	252						
ATOM 12342 0 HOH 255 86.628 29.295 53.611 1.00 28.08 W O ATOM 12343 0 HOH 256 102.111 48.926 69.771 1.00 28.02 W O ATOM 12344 0 HOH 257 117.835 65.790 61.089 1.00 30.23 W O ATOM 12345 0 HOH 258 105.286 61.859 63.757 1.00 33.92 W O ATOM 12346 0 HOH 259 86.743 64.218 34.930 1.00 28.91 W O ATOM 12347 0 HOH 260 105.249 47.160 40.635 1.00 20.28 W O	ATOM	12340	0			95. 637	65.687	28.739	1.00 22.07		
ATOM 12343 O HOH 256 102.111 48.926 69.771 1.00 28.02 W O ATOM 12344 O HOH 257 117.835 65.790 61.089 1.00 30.23 W O ATOM 12345 O HOH 258 105.286 61.859 63.757 1.00 33.92 W O ATOM 12346 O HOH 259 86.743 64.218 34.930 1.00 28.91 W O ATOM 12347 O HOH 260 105.249 47.160 40.635 1.00 20.28 W O							32. 347	36.665	1.00 21.89		0
ATOM 12344 0 HOH 257 117.835 65.790 61.089 1.00 30.23 W 0 ATOM 12345 0 HOH 258 105.286 61.859 63.757 1.00 33.92 W 0 ATOM 12346 0 HOH 259 86.743 64.218 34.930 1.00 28.91 W 0 ATOM 12347 0 HOH 260 105.249 47.160 40.635 1.00 20.28 W 0											
ATOM 12345 0 HOH 258 105.286 61.859 63.757 1.00 33.92 W O ATOM 12346 0 HOH 259 86.743 64.218 34.930 1.00 28.91 W O ATOM 12347 0 HOH 260 105.249 47.160 40.635 1.00 20.28 W O											
ATOM 12346 0 HOH 259 86.743 64.218 34.930 1.00 28.91 W O ATOM 12347 0 HOH 260 105.249 47.160 40.635 1.00 20.28 W O			-								
ATOM 12347 O HOH 260 105.249 47.160 40.635 1.00 20.28 W O											

	ATOM	12341	U	поп	Z00	105. 249				W	U

246/10/246

				FIC	3.4-	253			(Continued)
ATOM 12	348 0 349 0 350 0 351 0 352 0 353 0 354 0 355 0 356 0 357 0 358 0 358 0 359 0 360 0 361	HOH HOH HOH HOH HOH HOH HOH HOH HOH HOH	261 262 263 264 265 266 267 268 269 270 271 272 273 273	125. 748 73. 839 92. 355 102. 237 111. 596 76. 203 95. 406 71. 413 127. 938 122. 216 94. 659 77. 118 112. 752	77. 301 74. 279 54. 248 61. 200 65. 302 36. 588 54. 983 36. 734 49. 749 58. 021 59. 753 34. 975 32. 790	50. 793 32. 315 49. 336 14. 237 59. 180 32. 586 52. 304 46. 233 55. 356 31. 710 40. 284 51. 599 41. 771	1. 00 32. 51 1. 00 30. 75 1. 00 32. 87 1. 00 31. 77 1. 00 14. 35 1. 00 25. 41 1. 00 31. 62 1. 00 28. 42 1. 00 31. 01 1. 00 35. 14 1. 00 27. 37 1. 00 37. 45 1. 00 30. 32	W W W W W W W W W W W W W W W W W W W	0 0 0 0 0 0 0 0 0 0

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<150> US 60/398, 761

<151> 2002-07-29

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1				5					10					15		
cti	t gte	aco	ato	ato	ace	c gtg	g cc	g gtg	ggt	t cts	g ctg	g aac	c aaa	a gg	c aca	96
Leı	ı Vai	Thi	: Ile	e Ile	e Thi	r Val	Pro	o Val	l Va	l Lei	ı Leı	ı Ası	ı Lys	s Gl	y Thr	•
			20					25					30			
gat	gai	got	aca	gct	gae	c agi	cgo	c aaa	a aci	t tac	act	cta	a ac	t ga	t tac	144
Asp	Asp	Ala	Thr	Ala	ı Ası	Sei	Arg	g Lys	Thi	Tyr	Thr	Leu	ı Thi	r Ası	o Tyr	
		35					40					45				
t t a	aaa	aat	act	tat	aga	cte	aag	g tta	tac	t cc	: tta	aga	ı tgg	gati	t tca	192
Leu	Lys	Asn	Thr	Tyr	Are	g Leu	Lys	Let	ı Tyr	Ser	Leu	Arg	g Trp) Ile	e Ser	
	- 50					55					60					
gat	cat	gaa	tat	ctc	tac	aaa	caa	gaa	aat	aat	atc	ttg	gta	tto	aat	240
Asp	His	Glu	Tyr	Leu	Tyr	Lys	Gln	Glu	Asn	Asn	Ile	Leu	Val	Phe	e Asn	
65					70					75					80	
gc t	gaa	tat	gga	aac	agc	tca	gtt	ttc	ttg	gag	aac	agt	aca	ttt	gat	288
Ala	Glu	Tyr	Gly	Asn	Ser	Ser	Val	Phe	Leu	Glu	Asn	Ser	Thr	Phe	Asp	
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gag	itt	gga	cat	tct	atc	aat	gat	tat	tca	ata	tct	cct	gat	ggg	cag	336
Glu	Phe	Gly	His	Ser	.Ile	Asn	Asp	Туг	Ser	Ile	Ser	Pro	Asp	Gly	Gln	
			100					105					110			
ttt	att	ctc	tta	gaa	tac	aac	tac	gtg	aag	caa	tgg	agg	cat	tcc	tac	384
Phe	Ile _.	Leu	Leu	Glu	Tyr	Asn	Tyr	Val	Lys	Gln	Trp	Arg	His	Ser	Tyr	
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Thr	Ala	Ser	Tyr	Asp	Ile	Туг	Asp	Leu	Asn	Lys	Arg	Gln	Leu	Ile	Thr	
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Gly	His	Lys	Leu	Ala	Tyr	Val	Trp	Asn	Asn	Asp	Ile	Tyr	Val	Lys	He	
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Glu	Pro	Asn	Leu	Pro	Ser	Tyr	Arg	Ile	Thr	Trp	Thr	Gly	Lys	Glu	Asp	
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Ile	Ile	Tyr	Asn	Gly	Ile	Thr	Asp	Trp	Val	Tyr	Glu	Glu	Glu	Val	Phe	
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Ser	Ala	Tyr	Ser	Ala	Leu	Trp	Trp	Ser	Pro	Asn	Gly	Thr	Phe	Leu	Ala	
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tat	gcc	caa	ttt	aac	gac	aca	gaa	gtc	cca	ctt	att	gaa	. tac	tcc	ttc	720
Tyı	· Ala	Gln	Phe	Asn	Asp	Thr	Glu	Val	Pro	Leu	Ile	Glu	Tyr	Ser	Phe	
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Tyı	sei	Asp	Glu	Ser	Leu	Gln	Tyr	Pro	Lys	Thr	Val	Arg	y Val	Pro	Tyr	
				245)				250)				255	,	
cca	a aág	g gca	gga	a gct	gte	g aat	cca	act	gta	aag	g ttc	tti	gti	gta	ı aat	816
Pro	Lys	s Ala	Gly	/ Ala	a Val	Asn	Pro	Thr	Val	Lys	Phe	Phe	e Val	l Val	Asn	
			260)				265	j				270)		
aca	a ga	c tot	cto	c ago	c tca	gto	aco	aat	gca	act	tco	ata	a caa	a ato	act	864
Th	r Ası	ser	Le	ı Sei	r Ser	· Val	Thi	r Asr	ı Ala	Thi	Ser	· Ile	Gli	ı Ile	e Thr	
		275	5				280) .				285	5			
gc	t cc	t gc	ttc	t ats	g tte	g ata	ggg	g gat	t cac	tac	ttg	g tgi	t ga	t gts	g aca	912

Ala	Pro	Ala	Ser	Met	Leu	Ile	Gly	Asp	His	Tyr	Leu	Cys	Asp	Val	Thr	
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tgg	gca	aca	caa	. gaa	. aga	att	tci	ttg	cag	t gg	cto	agg	gagg	att	cag	960
Trp	Ala	Thr	Gln	Glu	Arg	He	Ser	Leu	Gln	Trp	Leu	Arg	, Arg	: Ile	Gln	
305					310					315					320	
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Asn	Tyr	Ser	Val	Met	Asp	He	Cys	Asp	Tyr	Asp	Glu	Ser	Ser	Gly	Arg	
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Trp	Asn	Cys	Leu	Val	Ala	Arg	Gln	His	Ile	Glu	Met	Ser	Thr	Thr	Gly	
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Trp	Val	Gly	Arg	Phe	Arg	Pro	Ser	Glu	Pro	His	Phe	Thr	Leu	Asp	Gly	
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aat	agc	ttc	tac	aag	atc	atc	agc	aat	gaa	gaa	ggt	tac	aga	cac	att	1152
Asn	Ser	Phe	Туг	Lys	Íle	Ile	Ser	Asn	Glu	Glu	Gly	Tyr	Arg	His	Ile	
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tgc	tat	ttc	caa	ata	gat	aaa	aaa	gac	tgc	aca	ttt	att	aca	aaa	ggc	1200
Cys	Tyr	Phe	Gln	Ile	Asp	Lys	Lys	Asp	Cys	Thr	Phe	Ile	Thr	Lys	Gly	
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Thr	Trp	Glu	Val	Ile	Gly	Ile	Glu	Ala	Leu	Thr	Ser	Asp	Tyr	Leu	Tyr	
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Tyr	Ile	Ser	Asn	Glu	Tyr	Lys	Gly	Me t	Pro	Gly	Gly	Arg	Asn	Leú	Tyr	
			420					425					430			
aaa	aic	caa	ctt	agt	gac	tat	aca	aaa	gtg	aca	tgc	ctc	agt	tgt	gag	1344

Lys	Ile	Gln	Leu	Ser	Asp	Tyr	Thr	Lys	Val	Thr	Cys	Leu	Ser	Cys	Glu	
		435					440					445				
ctg	aat	ccg	gaa	agg	tgt	cag	tac	tat	tct	gtg	tca	ttc	agt	aaa	gag	1392
Leu	Asn	Pro	Glu	Arg	Cys	Gln	Tyr	Tyr	Ser	Val	Ser	Phe	Ser	Lys	Glu	
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gcg	aag	tat	tat	cag	ctg	aga	tgt	tcc	ggt	cct	ggt	ctg	ccc	ctc	tat	1440
Ala	Lys	Tyr	Tyr	Gln	Leu	Arg	Cys	Ser	Gly	Pro	Gly	Leu	Pro	Leu	Tyr	
465					470					475					480	
ac t	cta	cac	agc	agc	gtg	aat	gat	aaa	ggg	ctg	aga	gtc	ctg	gaa	gac	1488
Thr	Leu	His	Ser	Ser	Val	Asn	Asp	Lys	Gly	Leu	Arg	Val	Leu	Glu	Asp	
				485					490					495		
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Lys	Leu	Asp	Phe	Ile	Ile	Leu	Asn	Glu	Thr	Lys	Phe	Trp	Tyr	Gln	Met	
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Asp	Val	Tyr	Ala	Gly	Pro	Cys	Ser	Gln	Lys	Ala	Asp	Thr	Val	Phe	Arg	
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Se	r Ph	e As	p Gly	y Ar	g Gly	/ Sei	Gly	y Tyi	Glr	ı Gly	y Asp	Lys	s Ile	Me	His	
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gc	a at	c aa	c aga	a aga	a ctg	g gga	aca	a ttt	gaa	gti	t gaa	gai	t caa	ati	gaa	1824
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gc	a gc	c ag	a ca	a tt	t tca	a aaa	ı atg	g gga	ttt	gtg	g gao	aac	aaa	cga	att	1872
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	610)				615	,				620)				
gc	a at	l lg	g gg(c tgg	g tca	tat	gga	ggg	tac	gta	aco	tca	ate	gto	ctg	1920
Ala	a Ile	e Tr	o Gly	/ Tr	Ser	Tyr	Gly	Gly	Tyr	Val	Thr	Ser	Met	Val	Leu	
629	5				630)				635	j				640	
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Gl	y Sei	Gly	y Ser	. Gl?	/ Val	Phe	Lys	Cys	Gly	Ile	. Ala	Val	Ala	Pro	Val	
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Gly	Thr	Ala	Asp	Asp	Asn	Val	His	Phe	Gln	Gln	Ser	Ala	Ġln	Ile	Ser	••
705					710					715					720	
aaa	gcc	cig	gtc	gat	gtt	gga	gtg	gat	ttc	cag	gca	aig	tgg	tat	act	2208

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7/11

Lys Ala Leu Val Asp Val Gly Val Asp Phe Gln Ala Met Trp Tyr Thr gat gaa gac cat gga ata gct agc agc aca gca cac caa cat ata tat Asp Glu Asp His Gly Ile Ala Ser Ser Thr Ala His Gln His Ile Tyr acc cac atg agc cac ttc ata aaa caa tgt ttc tct tta cct tag Thr His Met Ser His Phe Ile Lys Gln Cys Phe Ser Leu Pro

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<213 Homo sapiens

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	Ala	Glu	Tyr	Gly	Asn	Ser	Ser	Val	Phe	Leu	Glu	Asn	Ser	Thr	Phe	Asp
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	Glu	Phe	Gly	His	Ser	Ile	Asn	Asp	Tyr	Ser	Ile	Ser	Pro	Asp	Gly	Gln
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	Phe	Ile	Leu	Leu	Glu	Tyr	Asn	Tyr	Val	Lys	Gln	Trp	Arg	His	Ser	Tyr
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	Thr	Ala	Ser	Tyr	Asp	Ile	Tyr	Asp	Leu	Asn	Lys	Arg	Gln	Leu	Ile	Thr
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	Gly	His	Lys	Leu	Ala	Tyr	Val	Trp	Asn	Asn	Asp	Ile	Tyr	Val	Lys	Ile
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	Glu	Pro	Asn	Leu	Pro	Ser	Tyr	Arg	He	Thr	Trp	Thr	Gly	Lys	Glu	Asp
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	He	Ile	Tyr	Asn	Gly	He	Thr	Asp	Trp	Val	Tyr	Glu	Glu	Glu	Val	Phe
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	Tyr	Ser	Asp	Glu	Ser	Leu	Gln	Tyr	Pro	Lys	Thr	Val	Arg	Val	Pro	Tyr
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,	Ala	Pro	Ala	Ser	Met	Leu	Ile	Gly	Asp	His	Tyr	Leu	Cys	Asp	Val	Thr

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Asn	Tyr	Ser	Val	Met	Asp	Ile	Cys	Asp	Tyr	Asp	Glu	Ser	Ser	Gly	Arg
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Trp	Asn	Cys	Leu	Val	Ala	Arg	Gln	His	Ile	Glu	Met	Ser	Thr	Thr	Gly
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Trp	Val	Gly	Arg	Phe	Arg	Pro	Ser	Glu	Pro	His	Phe	Thr	Leu	Asp	Gly
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Cys	Tyr	Phe	Gln	Ile	Asp	Lys	Lys	Asp	Cys	Thr	Phe	Ile	Thr	Lys	Gly
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Thr	Trp	Glu	Val	Ile	Gly	Ile	Glu	Ala	Leu	Thr	Ser	Asp	Tyr	Leu	Tyr
				405					410					415	
Tyr	Ile	Ser	Asn	Glu	Tyr	Lys	Gly	Met	Pro	Gly	Gly	Arg	Asn	Leu	Tyr
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Lys	He	Gln	Leu	Ser	Asp	Tyr	Thr	Lys	Val	Thr	Cys	Leu	Ser	Cys	Glu
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Leu	Asn	Pro	Glu	Arg	Cys	Gln	Tyr	Tyr	Ser	Val	Ser	Phe	Ser	Lys	Glu
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Ala	Lys	Tyr	Tyr	Gln	Leu	Arg	Cys	Ser	Gly	Pro	Gly	Leu	Pro	Leu	Tyr
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Thr	Leu	His	Ser	Ser	Val	Asn	Asp	Lys	Gly	Leu	Arg	Val	Leu	Glu	Asp
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Asn	Ser	Ala	Leu	Asp	Lys	Met	Leu	Gln	Asn	Val	Gln	Met	Pro	Ser	Lys
			500					505					510		

Lys	Leu	Asp	Phe	Ile	He	Leu	Asn	Glu	Thr	Lys	Phe	Trp	Tyr	Gln	Met
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Ile	Leu	Pro	Pro	His	Phe	Asp	Lys	Ser	Lys	Lys	Tyr	Pro	Leu	Leu	Leu
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Asp	Val	Tyr	Ala	Gly	Pro	Cys	Ser	Gln	Lys	Ala	Asp	Thr	Val	Phe	Arg
545					550				•	555					560
Leu	Asn	Trp	Ala	Thr	Tyr	Leu	Ala	Ser	Thr	Glu	Asn	Ile	Ile	Val	Ala
				565					570					575	
Ser	Phe	Asp	Gly	Arg	Gly	Ser	Gly	Tyr	Gln	Gly	Asp	Lys	Ile	Met	His
			580					585					590		
Ala	Ile	Asn	Arg	Arg	Leu	Gly	Thr	Phe	Glu	Val	Glu	Asp	Gln	Ile	Glu
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Ser	Arg	Trp	Glu	Tyr	Tyr	Asp	Ser	Val	Tyr	Thr	Glu	Arg	Tyr	Met	Gly
			660					665					670		
Leu	Pro	Thr	Pro	Glu	Asp	Asn	Leu	Asp	His	Tyr	Arg	Asn	Ser	Thr	Val
		675					680					685			
Me t	Ser	Arg	Ala	Glu	Asn	Phe	Lys	Gln	Val	Glu	Tyr	Leu	Leu	Ile	His
	690					695			•		700				
Gly	Thr	Ala	Asp	Asp	Asn	Val	His	Phe	Gln	Gln	Ser	Ala	Gln	lle	Ser
705					710					715					720
Lys	Ala	Leu	Val	Asp	Val	Gly	Val	Asp	Phe	Gln	Ala	Met	Trp	Tyr	Thr

765

Asp Glu Asp His Gly Ile Ala Ser Ser Thr Ala His Gln His Ile Tyr Thr His Met Ser His Phe Ile Lys Gln Cys Phe Ser Leu Pro

760

755

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		FC1/UF U3,	7 09523
A. CLASSIF IPC 7	FICATION OF SUBJECT MATTER C12N9/48 C07K14/705 G01N23/2	20 GO1N33/573	
	International Patent Classification (IPC) or to both national classific	ation and IPC	
B. FIELDS			
Minimum do	cumentation searched (classification system followed by classification $C12N - C07K - G01N$	on symbols)	
	ion searched other than minimum documentation to the extent that s		
1	ata base consulted during the International search (name of data be ternal, WPI Data, PAJ, BIOSIS, EMBAS)
C. DOCUME	ENTS CONSIDERED TO BE RELEVANT		
Category °	Citation of document, with indication, where appropriate, of the re-	levant passages	Relevant to claim No.
χ	KABASHIMA T ET AL: "DIPEPTIDYL I	PEPTIDASE	1,2,6
Υ	IV FROM XANTHAMONAS MALTOPHILIA: SEQUENCING AND EXPRESSION OF THE GENE AND CHARACTERIZATION OF THE ENZYME" JOURNAL OF BIOCHEMISTRY, JAPANESI BIOCHEMICAL SOCIETY, TOKYO, JP, vol. 120, no. 6, December 1996 (pages 1111-1117, XP000973151 ISSN: 0021-924X figure 4 the whole document	ENZYME EXPRESSED	3-5, 14-20
X Funt	ner documents are listed in the continuation of box C.	Patent family members are listed	In annex.
"A" docume consid "E" earlier of filing d "L" docume which clation "O" docume other r "P" docume	ent which may throw doubts on priority claim(s) or is cited to establish the publication date of another no rother special reason (as specified) ent referring to an oral disclosure, use, exhibition or	*T* later document published after the Inte or priority date and not in conflict with cited to understand the principle or the invention invention. *X* document of particular relevance; the cannot be considered novel or cannot involve an inventive step when the document of particular relevance; the cannot be considered to involve an in document is combined with one or ments, such combination being obvious the art. *A* document member of the same patent	the application but every underlying the claimed Invention to econsidered to current is taken alone claimed invention ventive step when the one other such docu- us to a person skilled
	actual completion of the international search 9 November 2003	Date of mailing of the international second	arch report
	nalling address of the ISA European Patent Office, P.B. 5818 Patentlaan 2 NL - 2280 HV Rijswijk Tel. (+31-70) 340-2040, Tx. 31 651 epo nl, Fax: (+31-70) 340-3016	Authorized officer Bucka, A	

Form PCT/ISA/210 (second sheet) (July 1992)

Internation Application No
PCT/JP 03/09523

2/0- **	ation) DOCUMENTS CONSIDERED TO BE RELEVANT	101/01 03/09323
ategory *	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
1	ABBOTT CATHERINE A ET AL: "Binding to human dipeptidyl peptidase IV by adenosine deaminase and antibodies that inhibit ligand binding involves overlapping, discontinuous sites on a predicted beta propeller domain" EUROPEAN JOURNAL OF BIOCHEMISTRY, vol. 266, no. 3, December 1999 (1999-12), pages 798-810, XP002261851 ISSN: 0014-2956 the whole document	3-5, 14-20
Y	LAMBEIR A-M ET AL: "A prediction of DPP IV/CD26 domain structure from a physico-chemical investigation of dipeptidyl peptidase IV (CD26) from human seminal plasma" BIOCHIMICA ET BIOPHYSICA ACTA. PROTEIN STRUCTURE AND MOLECULAR ENZYMOLOGY, ELSEVIER, AMSTERDAM,, NL, vol. 1340, no. 2, 18 July 1997 (1997-07-18), pages 215-226, XP004281676 ISSN: 0167-4838 the whole document	3-5, 14-20
Y	MEDRANO F J ET AL: "Structure of proline iminopeptidase from Xanthomonas campestris pv. citri: A prototype for the prolyl oligopeptidase family" EMBO (EUROPEAN MOLECULAR BIOLOGY ORGANIZATION) JOURNAL, vol. 17, no. 1, 2 January 1998 (1998-01-02), pages 1-9, XP002261745 ISSN: 0261-4189 the whole document	3-5, 14-20
A	POLGAR L: "The prolyl oligopeptidase family" CMLS CELLULAR AND MOLECULAR LIFE SCIENCES, BIRKHAUSER VERLAG, BASEL, CH, vol. 59, no. 2, February 2002 (2002-02), pages 349-362, XP002219152 ISSN: 1420-682X the whole document	1-6, 14-20
Α	FULOP V ET AL: "Prolyl oligopeptidase: An unusual beta-propeller domain regulates proteolysis" CELL, CELL PRESS, CAMBRIDGE, NA, US, vol. 94, no. 2, 24 July 1998 (1998-07-24), pages 161-170, XP002221331 ISSN: 0092-8674 the whole document	1-6, 14-20

Internation Application No
PCT/JP 03/09523

C.(Continua	ation) DOCUMENTS CONSIDERED TO BE RELEVANT	
Category °	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
A	AUGUSTYNS K ET AL: "THE UNIQUE PROPERTIES OF DIPEPTIDYL-PEPTIDASE IV (DPP IV/CD26) AND THE THERAPEUTIC POTENTIAL OF DPP IV INHIBITORS" CURRENT MEDICINAL CHEMISTRY, BENTHAM SCIENCE PUBLISHERS BV, BE, vol. 6, no. 4, 1999, pages 311-327, XP000870290 ISSN: 0929-8673 the whole document	1-6, 14-20
P, X	ENGEL MICHAEL ET AL: "The crystal structure of dipeptidyl peptidase IV (CD26) reveals its functional regulation and enzymatic mechanism." PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES, vol. 100, no. 9, 29 April 2003 (2003-04-29), pages 5063-5068, XP002261746 April 29, 2003 ISSN: 0027-8424 (ISSN print) the whole document	1-6, 14-20
P,X	RASMUSSEN HANNE B ET AL: "Crystal structure of human dipeptidyl peptidase IV/CD26 in complex with a substrate analog." NATURE STRUCTURAL BIOLOGY, vol. 10, no. 1, January 2003 (2003-01), pages 19-25, XP001168693 ISSN: 1072-8368 (ISSN print) the whole document	1-6, 14-20
P,X	HIRAMATSU HAJIME ET AL: "The structure and function of human dipeptidyl peptidase IV, possessing a unique eight-bladed beta-propeller fold." BIOCHEMICAL AND BIOPHYSICAL RESEARCH COMMUNICATIONS, vol. 302, no. 4, 21 March 2003 (2003-03-21), pages 849-854, XP002261748 ISSN: 0006-291X the whole document	1-6, 14-20

Internation Application No
PCT/JP 03/09523

	rc1/0r 03/09523		
	ation) DOCUMENTS CONSIDERED TO BE RELEVANT	Too	levant to claim No.
Category *	Citation of document, with indication, where appropriate, of the relevant passages	ne ne	IV VIAMII NV.
P,X	OEFNER CHRISTIAN ET AL: "High-resolution structure of human apo dipeptidyl peptidase IV/CD26 and its complex with 1-'('2-'(5-iodopyridin-2-yl)amino!-ethyl!a mino)- acetyl!-2-cyano-(S)-pyrrolidine." ACTA CRYSTALLOGRAPHICA. SECTION D, BIOLOGICAL CRYSTALLOGRAPHY. DENMARK JUL 2003, vol. 59, no. Pt 7, July 2003 (2003-07), pages 1206-1212, XP008024791 ISSN: 0907-4449 the whole document		1-6, 14-20

International application No. PCT/JP 03/09523

INTERNATIONAL SEARCH REPORT

Box I Observations where certain claims were found unsearchable (Continuation of Item 1 of Irrst sheet)			
This international Search Report has not been established in respect of certain claims under Article 17(2)(a) for the following reasons:			
1. X Claims Nos.: 7-13 22-24 because they relate to subject matter not required to be searched by this Authority, namely: see FURTHER INFORMATION sheet PCT/ISA/210			
2. X Claims Nos.: because they relate to parts of the International Application that do not comply with the prescribed requirements to such an extent that no meaningful International Search can be carried out, specifically: see FURTHER INFORMATION sheet PCT/ISA/210			
3. Claims Nos.: because they are dependent claims and are not drafted in accordance with the second and third sentences of Rule 6.4(a).			
Box II Observations where unity of invention is lacking (Continuation of item 2 of first sheet)			
This International Searching Authority found multiple inventions in this international application, as follows:			
As all required additional search fees were timely paid by the applicant, this International Search Report covers all searchable claims.			
2. As all searchable claims could be searched without effort justifying an additional fee, this Authority did not invite payment of any additional fee.			
3. As only some of the required additional search fees were timely paid by the applicant, this International Search Report covers only those claims for which fees were paid, specifically claims Nos.:			
A. No required additional search fees were timely paid by the applicant. Consequently, this international Search Report is restricted to the invention first mentioned in the claims; it is covered by claims Nos.:			
Remark on Protest The additional search fees were accompanied by the applicant's protest. No protest accompanied the payment of additional search fees.			

FURTHER INFORMATION CONTINUED FROM PCT/ISA/ 210

Continuation of Box I.1

Claims Nos.: 7-13, 22-24

Concerning claims 7 to 13 and 22 to 24 applicant's attention is drawn to Rule 39.1(v) PCT.

The subject-matter of claims 7 to 13 and 22 to 24 refers only to the presentation of structural information and is not regarded as patentable invention within the meaning of Rule 39.1(v) PCT. This information is disclosed e. g. as the atomic coordinates listings (or Tables) of a model, their use in a non-technical method, or said information is stored on a diskette/computer.

Thus, the above mentioned claims will not be searched in accordance with Article 17(2)(a)(i) PCT.

Continuation of Box I.2

Claims Nos.: 21

Present claim 21 relates to a product, i. e. an "effector", defined by reference to a desirable characteristic or property, namely as being an effector of dipeptidyl peptidase IV.

The claim covers all products having this characteristic or property, whereas the application provides no support within the meaning of Article 6 PCT and no disclosure within the meaning of Article 5 PCT of any such products. In the present case, the claim so lacks support, and the application so lacks disclosure, that a meaningful search of the claim is impossible.

Independent of the above reasoning, the claim also lacks clarity (Article 6 PCT). An attempt is made to define the product by reference to a result to be achieved. Again, this lack of clarity in the present case is such as to render a meaningful search over the whole of the claimed scope impossible.

Consequently, no search has been carried out under the provisions of Article 17(2)(a)(ii) PCT.

The applicant's attention is drawn to the fact that claims, or parts of claims, relating to inventions in respect of which no international search report has been established need not be the subject of an international preliminary examination (Rule 66.1(e) PCT). The applicant is advised that the EPO policy when acting as an International Preliminary Examining Authority is normally not to carry out a preliminary examination on matter which has not been searched. This is the case irrespective of whether or not the claims are amended following receipt of the search report or during any Chapter II procedure.